LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SAMPLE-1-GRAB

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029717.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.198	385	393	400	rBV	401108	609153	14.07%	1.050%
2	5.881	502	509	515	rBV5	23299	46798	1.08%	0.081%
3	6.592	626	630	635	rVB	58368	88050	2.03%	0.152%
4	6.781	651	662	676	rBV	361078	704867	16.28%	1.215%
5	7.592	792	800	807	rBV3	281576	506087	11.69%	0.872%
6	7.822	835	839	857	rVB3	37021	89817	2.08%	0.155%
7	7.986	861	867	877	rVB2	46012	94765	2.19%	0.163%
8	8.128	887	891	896	rVV	39676	64068	1.48%	0.110%
9	8.263	905	914	922	rVB3	39185	93111	2.15%	0.161%
10	8.357	922	930	934	rBV2	25747	46364	1.07%	0.080%
11	8.692	978	987	990	rBV2	55527	95615	2.21%	0.165%
12	8.745	990	996	1006	rVV2	336047	808515	18.68%	1.394%
13	8.822	1006	1009	1018	rVB	28637	51991	1.20%	0.090%
14	8.939	1019	1029	1038	rBV3	25423	88072	2.03%	0.152%
15	9.216	1072	1076	1081	rVV	33209	57186	1.32%	0.099%
16	9.275	1081	1086	1095	rVB	35977	67498	1.56%	0.116%
17	9.475	1112	1120	1124	rBV5	23482	46126	1.07%	0.080%
18	9.663	1143	1152	1158	rVB4	59358	122093	2.82%	0.210%
19	9.780	1167	1172	1176	rBV2	30875	51319	1.19%	0.088%
20	9.851	1181	1184	1190	rVV2	28657	47115	1.09%	0.081%
21	10.375	1262	1273	1278	rBV	342590	645421	14.91%	1.113%
22	10.422	1278	1281	1289	rVV6	42970	98428	2.27%	0.170%
23	10.492	1289	1293	1298	rVB	29782	45211	1.04%	0.078%
24	10.792	1333	1344	1351	rBV3	37472	82120	1.90%	0.142%
25	11.004	1374	1380	1383	rBV3	33916	61010	1.41%	0.105%
26	11.292	1423	1429	1436	rVB5	36438	70145	1.62%	0.121%
27	11.404	1443	1448	1457	rBV4	29512	71816	1.66%	0.124%
28	11.569	1468	1476	1485	rBV	90717	182099	4.21%	0.314%
29	11.827	1512	1520	1525	rBV2	115628	241763	5.59%	0.417%
30	11.880	1525	1529	1545	rVB	130245	292651	6.76%	0.504%
31	12.863	1687	1696	1705	rBV	686107	1053718	24.34%	1.816%
32	13.074	1728	1732	1738	rBV	43720	60898	1.41%	0.105%
33	13.721	1836	1842	1848	rBV4	40812	94797	2.19%	0.163%
34	14.068	1896	1901	1910	rVB	100823	140079	3.24%	0.241%
35	14.210	1919	1925	1928	rVV	1471641	1982290	45.80%	3.417%
36	14.245	1928	1931	1940	rVV2	541321	794730	18.36%	1.370%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SAMPLE-1-GRAB

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.845	2023	2033	2041	rBV4	22493	72914	1.68%	0.126%
38	15.257	2098	2103	2109	rBV	120158	160997	3.72%	0.278%
39	15.639	2164	2168	2173	rVB	52841	68482	1.58%	0.118%
40	15.698	2173	2178	2181	rBV	233186	348243	8.05%	0.600%
41	15.745	2181	2186	2195	rVV2	584233	1032513	23.85%	1.780%
42	15.927	2208	2217	2222	rBV	196337	297944	6.88%	0.514%
43	15.998	2222	2229	2232	rVV	1066345	1523796	35.20%	2.627%
44	16.033	2232	2235	2240	rVV	2599609	3071998	70.97%	5.296%
45	16.092	2240	2245	2249	rVV	2236638	3041675	70.27%	5.243%
46	16.151	2249	2255	2261	rVV2	2155815	4328364	100.00%	7.461%
47	16.209	2261	2265	2269	rVV2	2206437	3427067	79.18%	5.908%
48	16.256	2269	2273	2277	rVV	1423270	2046330	47.28%	3.528%
49	16.333	2277	2286	2288	rVV2	956746	2162694	49.97%	3.728%
50	16.357	2288	2290	2294	rVV	974245	1119047	25.85%	1.929%
51	16.409	2294	2299	2306	rVV3	2079311	4112469	95.01%	7.089%
52	16.480	2306	2311	2314	rVV	2478182	3444767	79.59%	5.938%
53	16.515	2314	2317	2320	rVV2	719080	1186194	27.41%	2.045%
54	16.551	2320	2323	2330	rVB2	1541831	2054447	47.46%	3.542%
55	16.609	2330	2333	2338	rVB5	31639	47343	1.09%	0.082%
56	16.692	2342	2347	2351	rBV2	113343	181895	4.20%	0.314%
57	16.756	2353	2358	2361	rVV3	122606	215561	4.98%	0.372%
58	16.804	2361	2366	2371	rVV	136312	278796	6.44%	0.481%
59	16.851	2371	2374	2377	rVV	65684	102541	2.37%	0.177%
60	16.886	2377	2380	2383	rVV2	85414	128183	2.96%	0.221%
61	16.915	2383	2385	2393	rVV2	56523	82690	1.91%	0.143%
62	16.992	2393	2398	2408	rVB	679630	982324	22.70%	1.693%
63	17.145	2421	2424	2427	rBV2	41291	60699	1.40%	0.105%
64	17.186	2428	2431	2436	rVV4	43723	88936	2.05%	0.153%
65	17.227	2436	2438	2442	rVV2	46468	58820	1.36%	0.101%
66	17.304	2446	2451	2457	rVB4	108950	203999	4.71%	0.352%
67	17.362	2457	2461	2465	rBV	114071	186489	4.31%	0.321%
68	17.474	2476	2480	2483	rBV	111341	143756	3.32%	0.248%
69	17.515	2483	2487	2489	rVV3	47243	63397	1.46%	0.109%
70	17.556	2489	2494	2501	rVB	1156727	1504094	34.75%	2.593%
71	17.709	2515	2520	2527	rVB	437219	588753	13.60%	1.015%
72	17.909	2548	2554	2560	rBV	711543	1066580	24.64%	1.839%
73	17.968	2560	2564	2569	rVB	112564	162210	3.75%	0.280%
74	18.239	2606	2610	2614	rBV2	54108	81332	1.88%	0.140%
75	18.439	2641	2644	2650	rVB2	38723	70015	1.62%	0.121%
76	18.880	2715	2719	2724	rBV	262343	313310	7.24%	0.540%

LSC Area Percent Report

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Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SAMPLE-1-GRAB

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	18.980	2731	2736	2741	rBV	1507569	1820139	42.05%	3.138%
78	19.015	2741	2742	2746	rVV	49459	49003	1.13%	0.084%
79	19.062	2746	2750	2752	rVV	46366	80410	1.86%	0.139%
80	19.103	2752	2757	2764	rVB5	94398	222042	5.13%	0.383%
81	19.186	2767	2771	2778	rVV2	158301	227890	5.27%	0.393%
82	19.450	2813	2816	2822	rVB2	95828	124127	2.87%	0.214%
83	19.627	2841	2846	2852	rBV	1255871	1564234	36.14%	2.696%
84	19.997	2905	2909	2916	rVB	222276	261371	6.04%	0.451%
85	20.156	2932	2936	2942	rVB	352619	382438	8.84%	0.659%
86	20.909	3061	3064	3071	rVB	136912	177144	4.09%	0.305%
87	20.986	3074	3077	3083	rVB2	161524	226606	5.24%	0.391%
88	21.103	3093	3097	3100	rBV	443156	504561	11.66%	0.870%
89	21.133	3100	3102	3105	rVV	197168	187534	4.33%	0.323%
90	21.174	3105	3109	3114	rVV	918727	1119756	25.87%	1.930%
91	23.356	3474	3480	3487	rVB2	665349	1255471	29.01%	2.164%

Sum of corrected areas: 58010176

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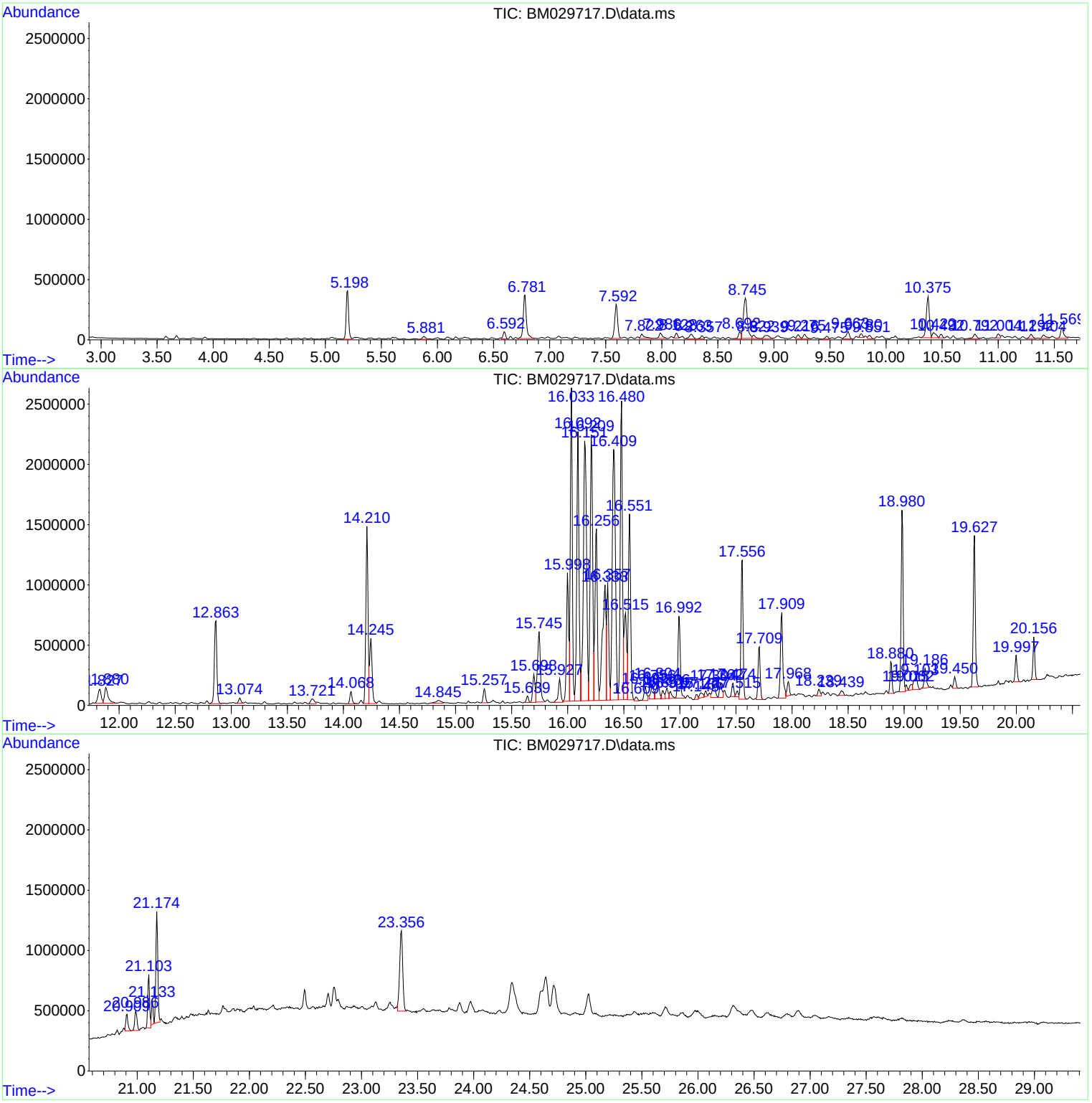
Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
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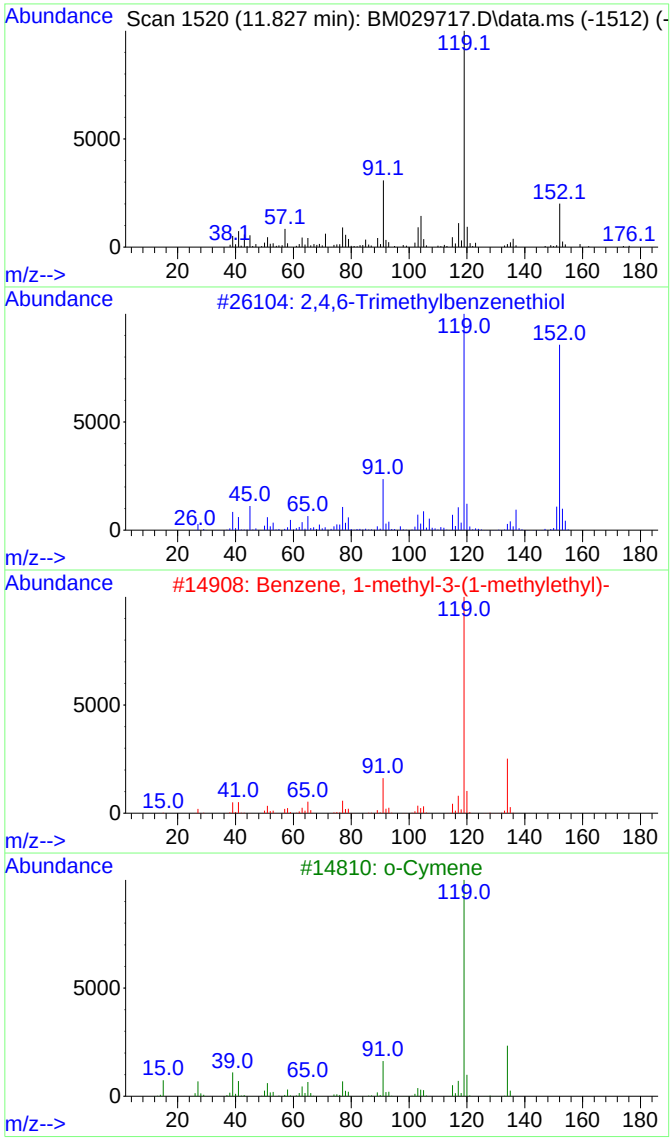
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

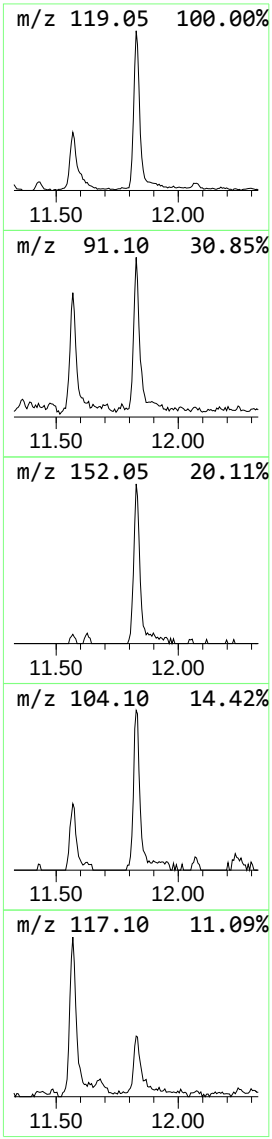
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4,6-Trimethylbenzenethiol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	7.49 ng	241763	Naphthalene-d8	10.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Trimethylbenzenethiol	152	C9H12S	001541-10-2	80
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	76
3	o-Cymene	134	C10H14	000527-84-4	76
4	p-Cymene	134	C10H14	000099-87-6	76
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
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Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

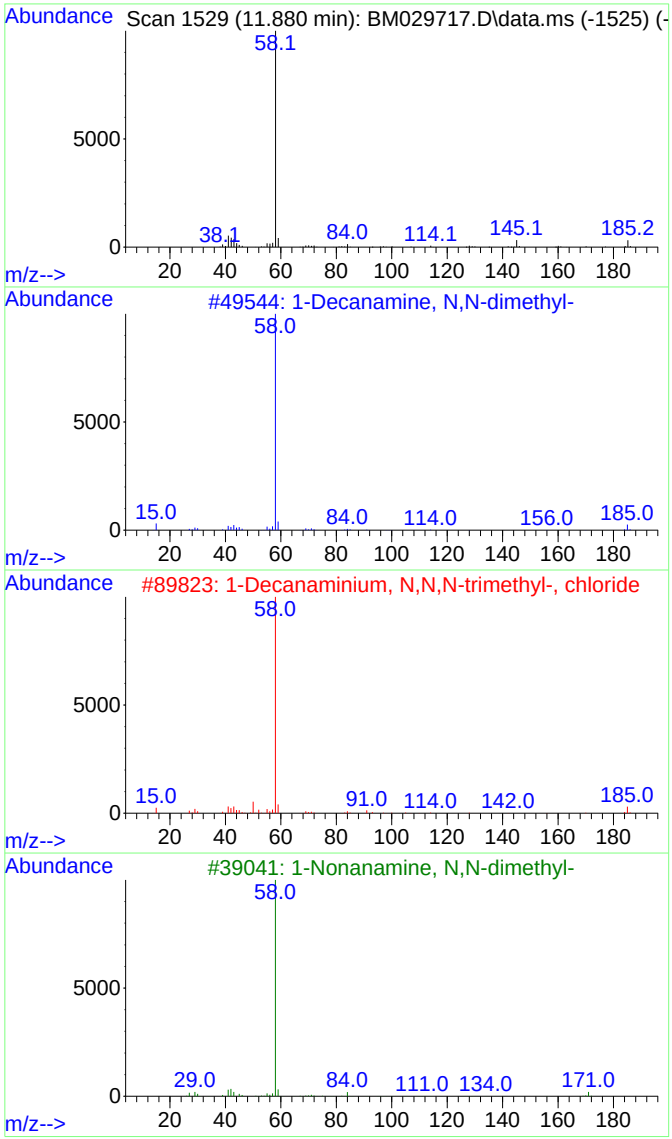
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

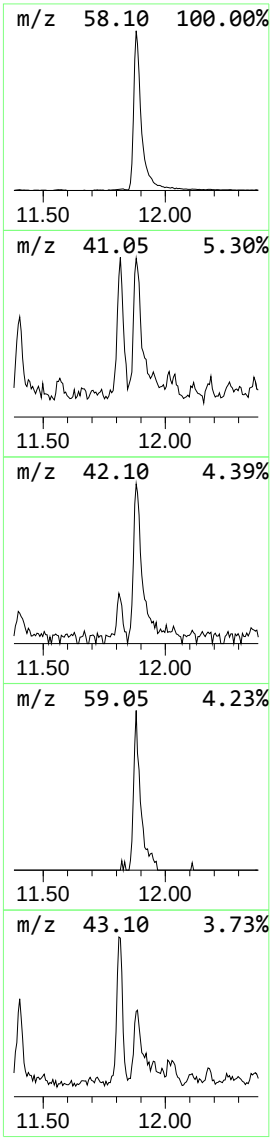
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Decanamine, N,N-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	9.07 ng	292651	Naphthalene-d8	10.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanamine, N,N-dimethyl-	185	C12H27N	001120-24-7	86
2	1-Decanaminium, N,N,N-trimethyl-...	235	C13H30ClN	010108-87-9	78
3	1-Nonanamine, N,N-dimethyl-	171	C11H25N	017373-27-2	72
4	1-Heptanamine, N,N-dimethyl-	143	C9H21N	005277-11-2	72
5	N,N-Dimethyl-2-tert-butoxyethyla...	145	C8H19NO	071126-61-9	72





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

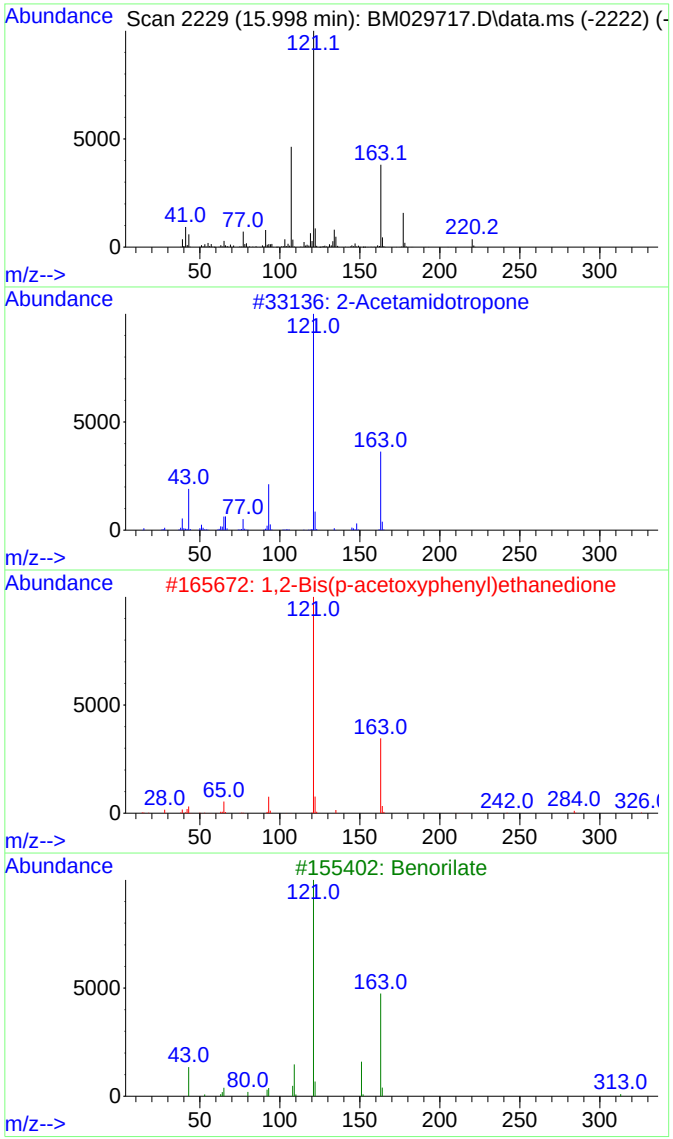
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

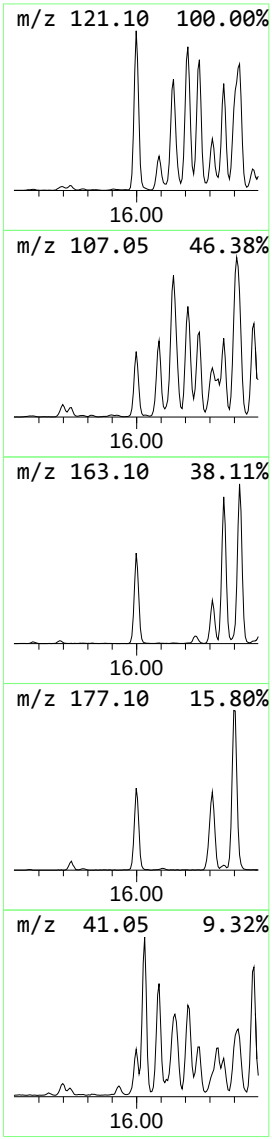
****

Peak Number 3 2-Acetamidotropone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	31.02 ng	1523800	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Acetamidotropone	163	C9H9NO2	006422-12-4	50
2	1,2-Bis(p-acetoxyphenyl)ethanedione	326	C18H14O6	093655-79-9	50
3	Benorilate	313	C17H15NO5	005003-48-5	40
4	2-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	000122-84-9	38
5	N-Allyl-p-hydroxybenzamide	177	C10H11NO2	090921-72-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
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Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

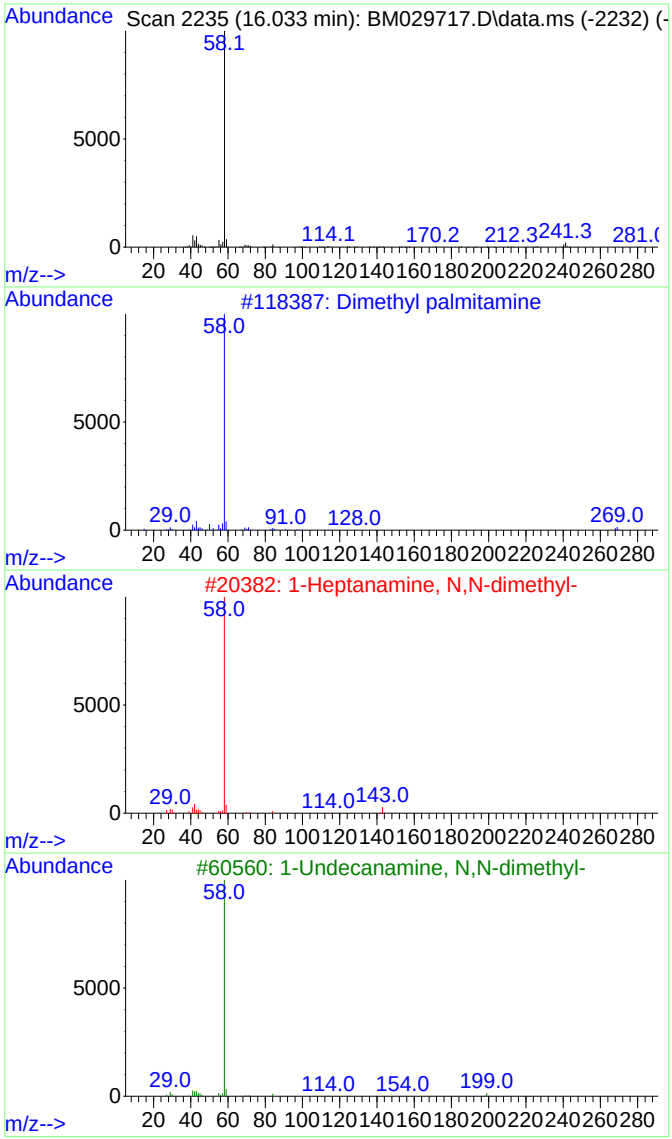
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

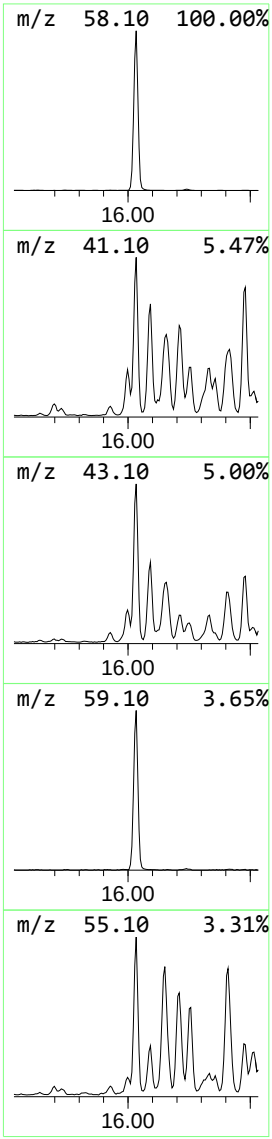
****

Peak Number 4 Dimethyl palmitamine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	62.55 ng	3072000	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl palmitamine	269	C18H39N	000112-69-6	72
2	1-Heptanamine, N,N-dimethyl-	143	C9H21N	005277-11-2	72
3	1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	72
4	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	72
5	1-Tridecanamine, N,N-dimethyl-	227	C15H33N	017373-29-4	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

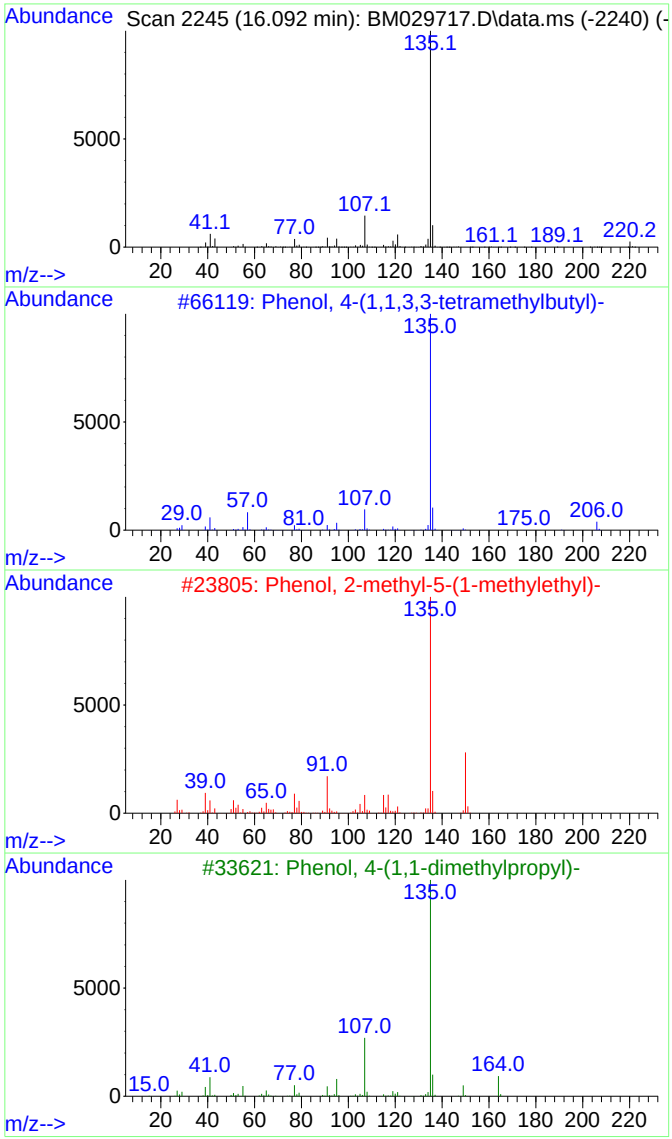
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

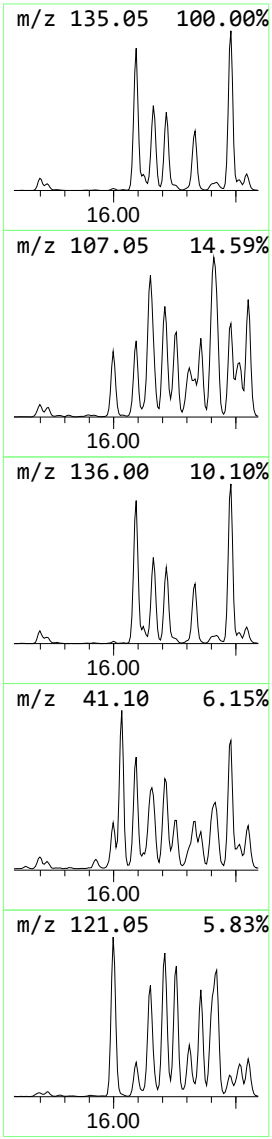
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.092	61.93 ng	3041680	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	78
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
4	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	64
5	1,2-Benzenediol, o-(4-methoxyben...	362	C22H18O5	1000325-99-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SAMPLE-1-GRAB

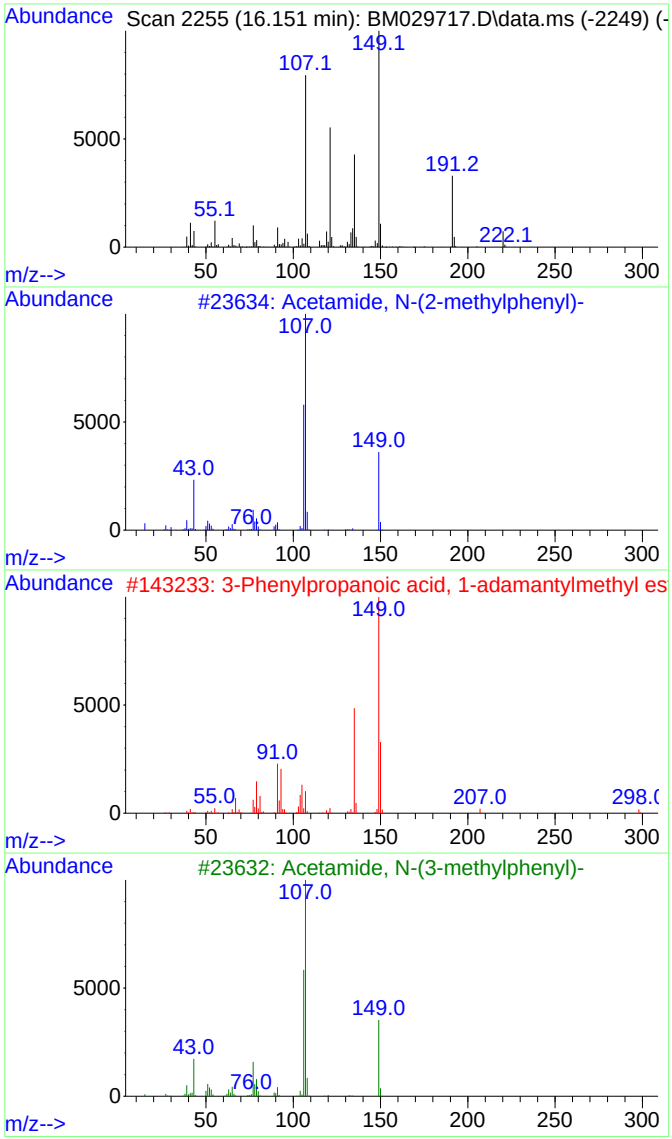
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

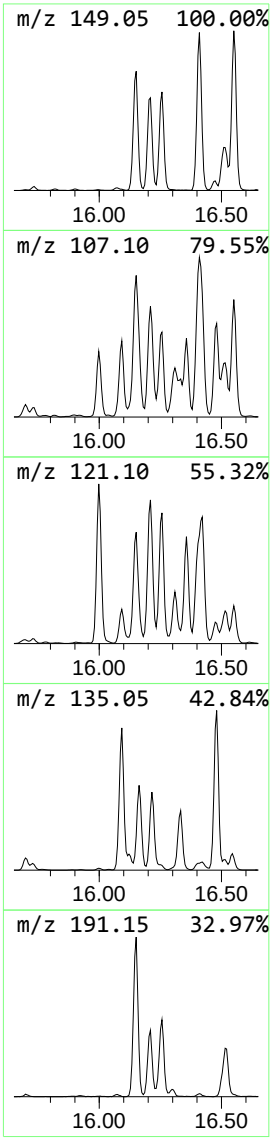
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown16.151 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.151	88.13 ng	4328360	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	43
2	3-Phenylpropanoic acid, 1-adaman...	298	C20H26O2	1000282-93-6	38
3	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	38
4	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	38
5	Phthalic acid, 2,4-dimethylpent-...	306	C18H26O4	1000356-84-2	35





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Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

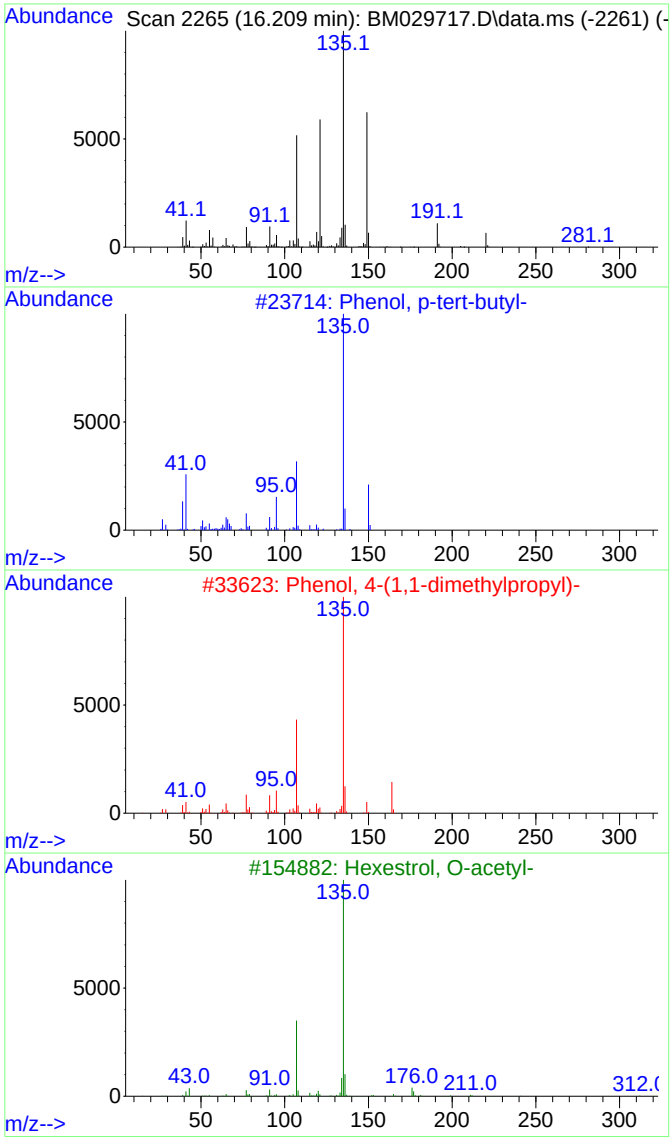
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

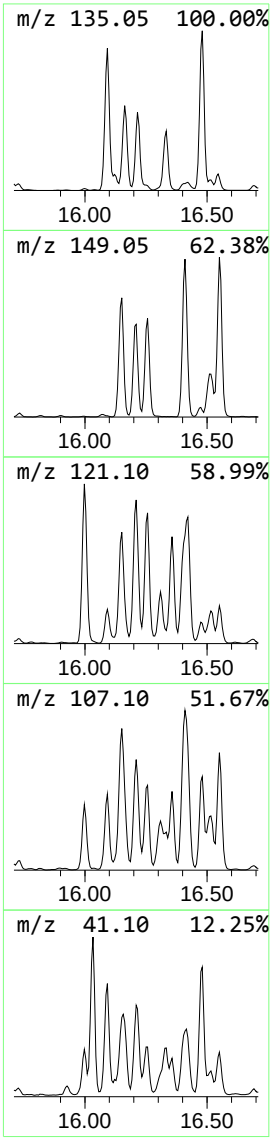
****

Peak Number 7 Phenol, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.209	69.77 ng	3427070	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	58
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	50
3	Hexestrol, O-acetyl-	312	C20H24O3	1000374-87-8	50
4	Hexestrol	270	C18H22O2	005635-50-7	47
5	Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	47





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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

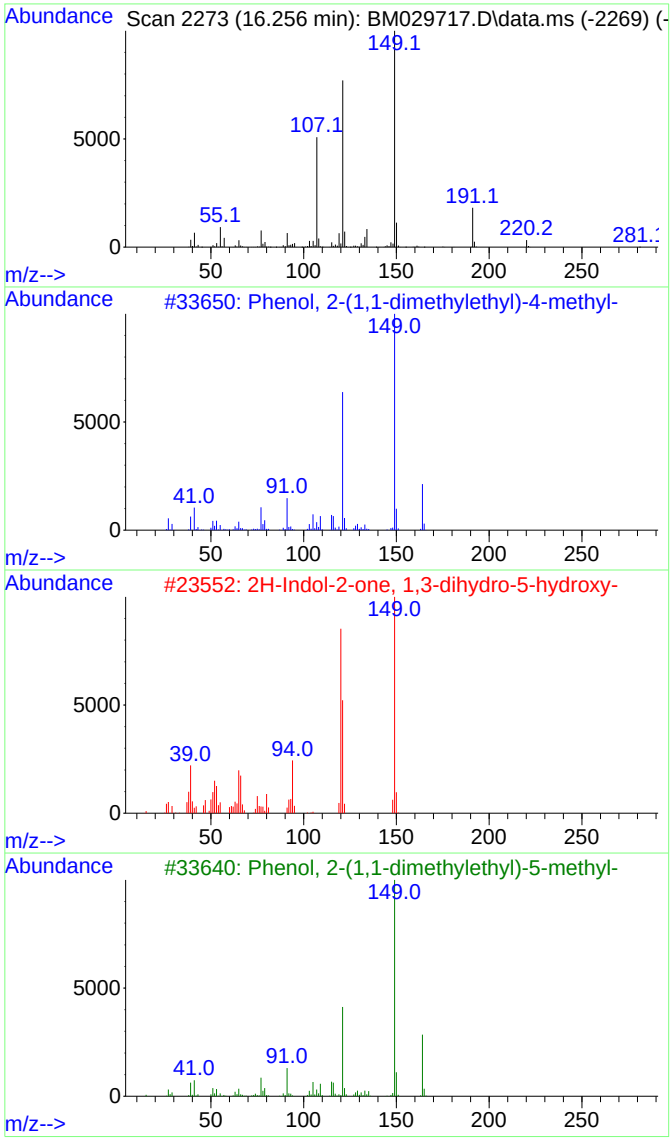
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

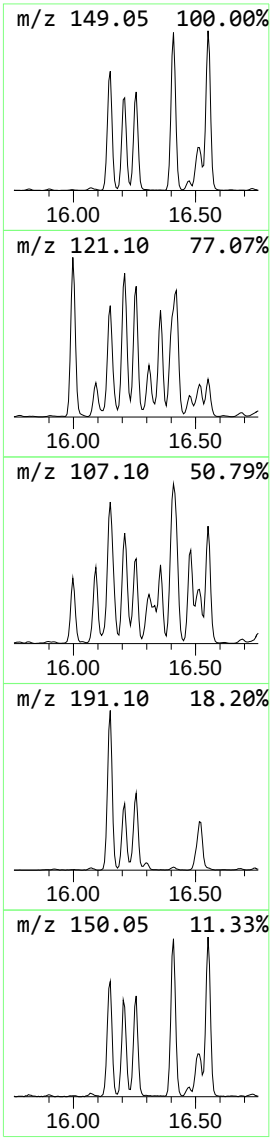
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 2-(1,1-dimethylethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.256	41.66 ng	2046330	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	59
2	2H-Indol-2-one, 1,3-dihydro-5-hy...	149	C8H7NO2	003416-18-0	53
3	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	45
4	Phenol, 4-(1,1-dimethylethyl)-2-...	164	C11H16O	000098-27-1	35
5	Phthalic acid, hept-4-yl propyl ...	306	C18H26O4	1000356-78-2	35





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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SAMPLE-1-GRAB

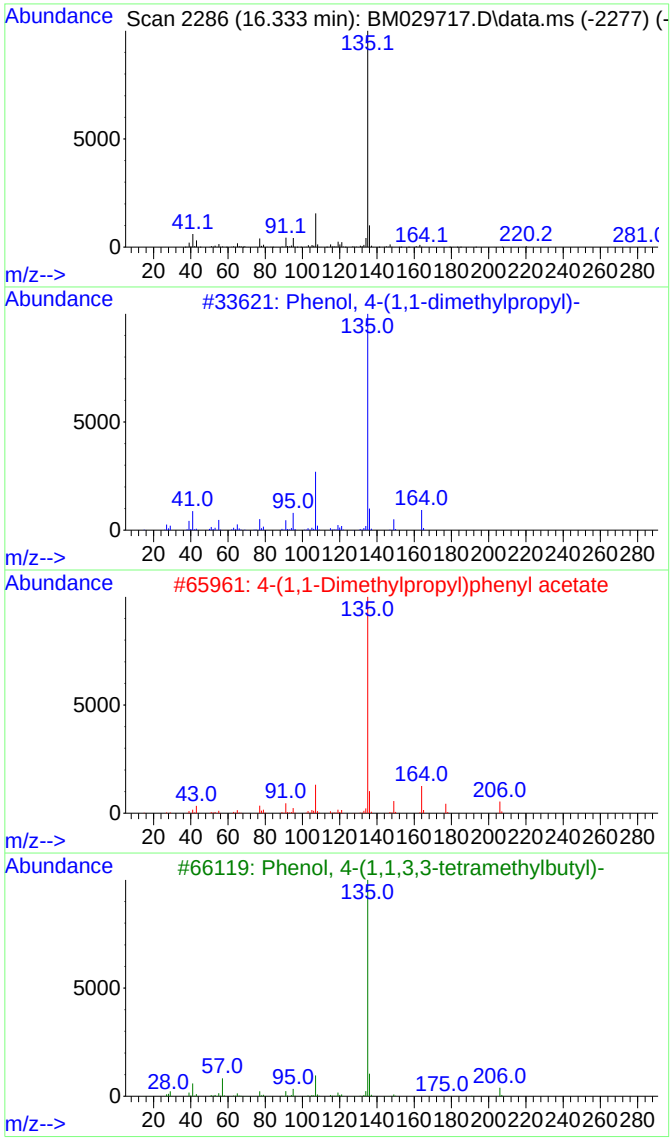
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

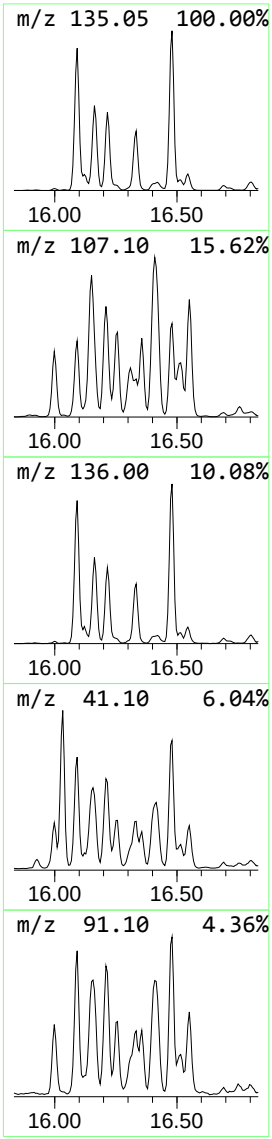
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 4-(1,1-dimethylprop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	44.03 ng	2162690	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
2	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
3	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
4	m-Anisic acid, cyclobutyl ester	206	C12H14O3	1000292-25-0	64
5	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	64





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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SAMPLE-1-GRAB

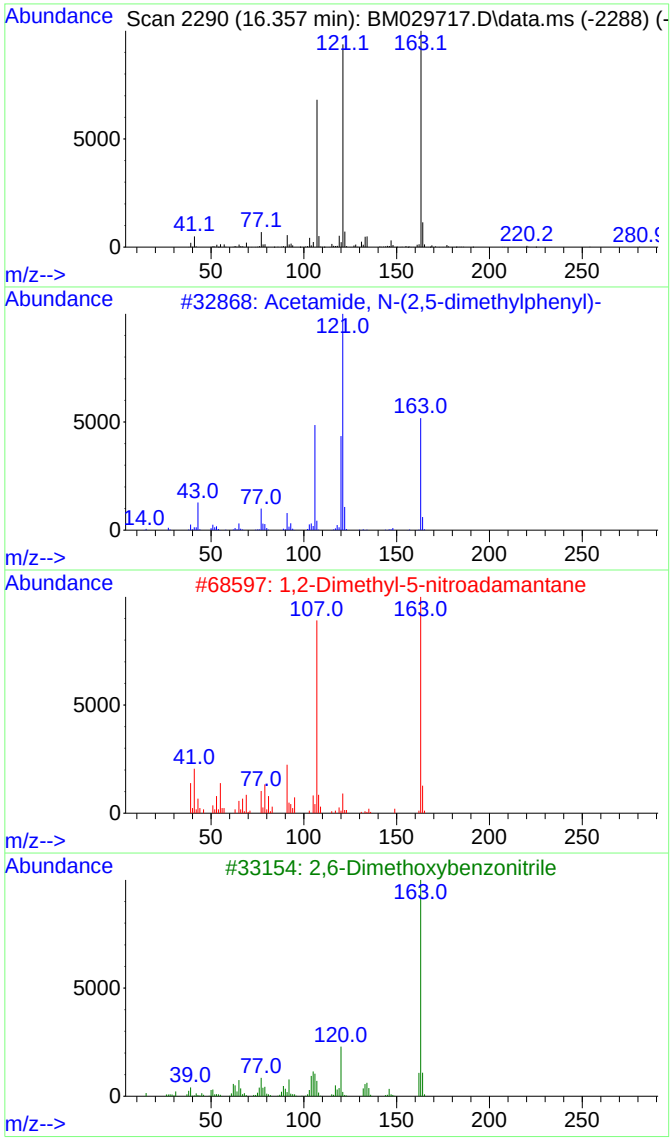
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

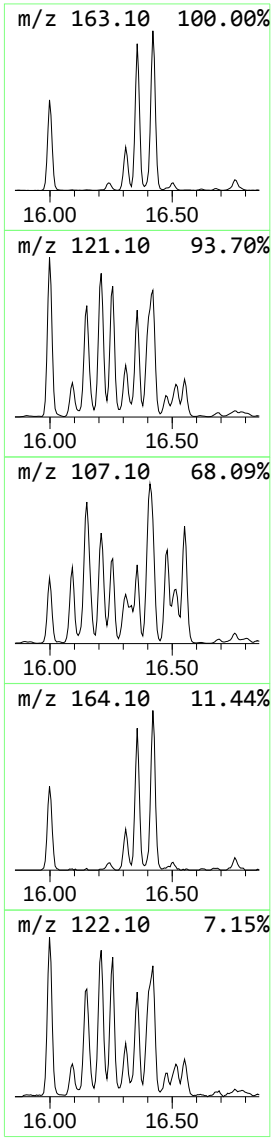
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Acetamide, N-(2,5-dimethylp... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.357	22.78 ng	1119050	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2,5-dimethylphenyl)-	163	C10H13NO	002050-44-4	53
2	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	47
3	2,6-Dimethoxybenzonitrile	163	C9H9NO2	016932-49-3	35
4	Carbonic acid, ethyl 4-isopropyl...	208	C12H16O3	1000331-34-2	27
5	1,2-Hexanediol, 1,2-diphenyl-	270	C18H22O2	080475-19-0	25





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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SAMPLE-1-GRAB

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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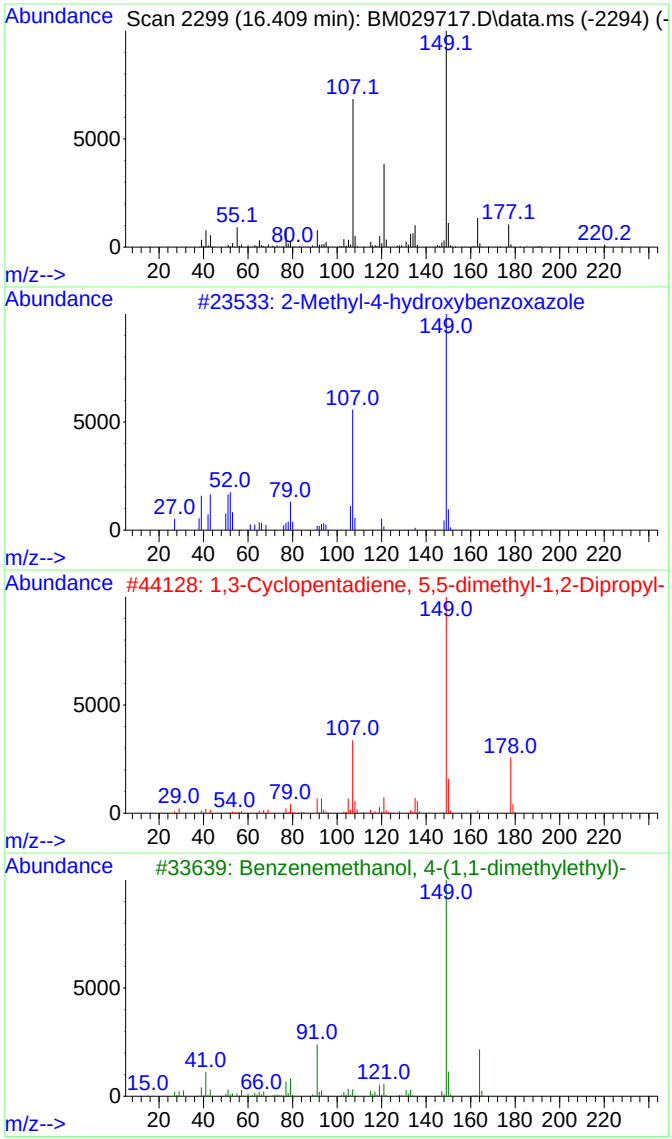
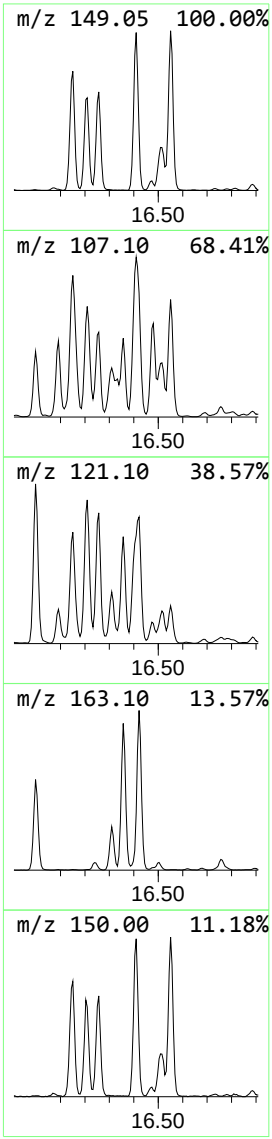
Peak Number 11 2-Methyl-4-hydroxybenzoxazole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.409	83.73 ng	4112470	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	53
2	1,3-Cyclopentadiene, 5,5-dimethy...	178	C13H22	1000163-88-0	50
3	Benzenemethanol, 4-(1,1-dimethyl...	164	C11H16O	000877-65-6	50
4	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	49
5	3-Ethoxy-4-hydroxyphenylacetonit...	177	C10H11NO2	205748-01-2	43





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Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

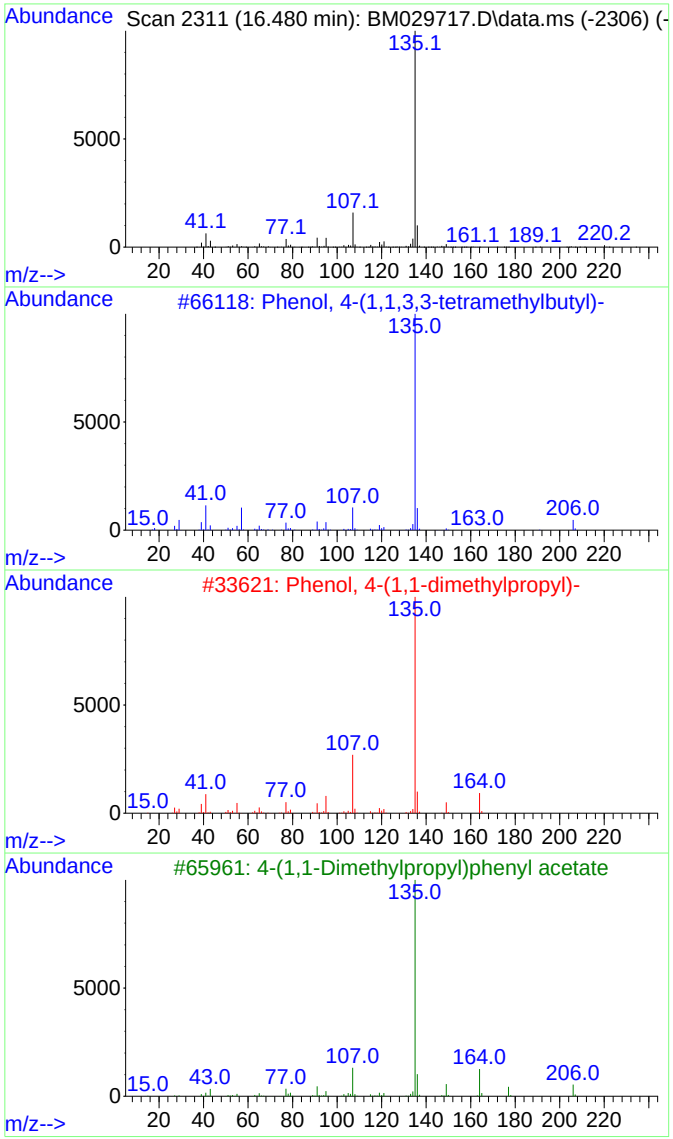
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

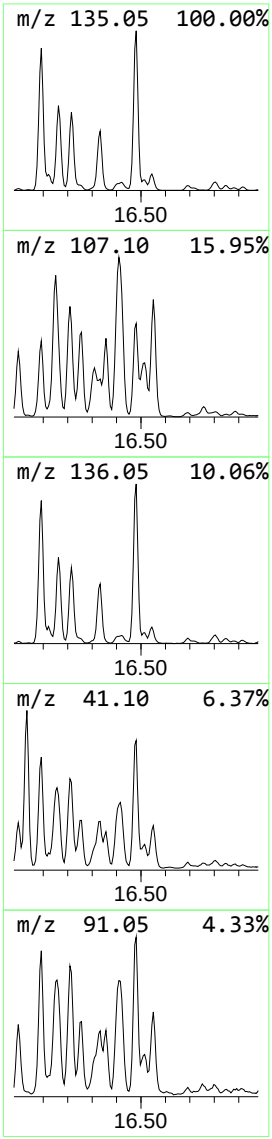
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 4-(1,1-Dimethylpropyl)pheny... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	70.14 ng	3444770	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
3	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
4	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	64
5	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	64





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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SAMPLE-1-GRAB

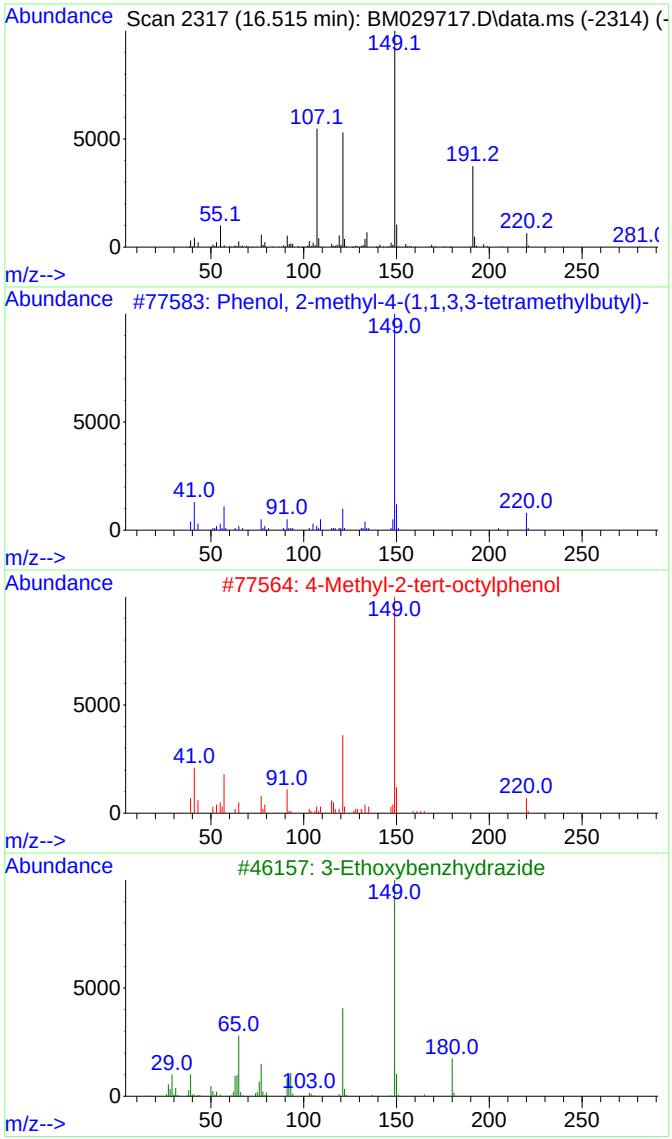
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

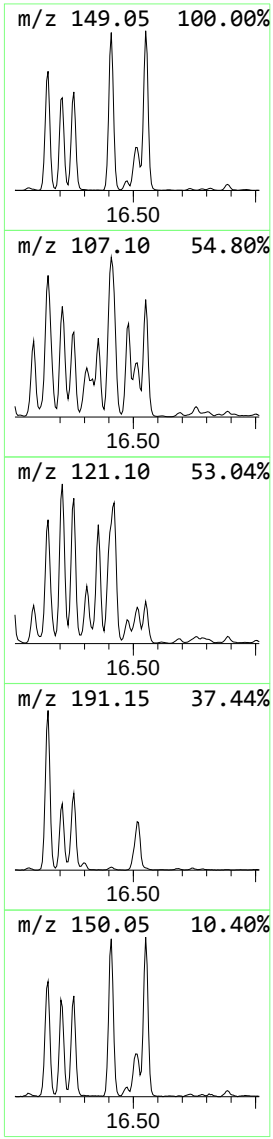
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 unknown16.515 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.515	24.15 ng	1186190	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	49
2	4-Methyl-2-tert-octylphenol	220	C15H24O	004979-46-8	47
3	3-Ethoxybenzhydrazide	180	C9H12N2O2	027830-16-6	43
4	1,2-propanedione,1-(3,4-methylen...	192	C10H8O4	1000378-93-0	43
5	2H-Indol-2-one, 1,3-dihydro-5-hy...	149	C8H7NO2	003416-18-0	43





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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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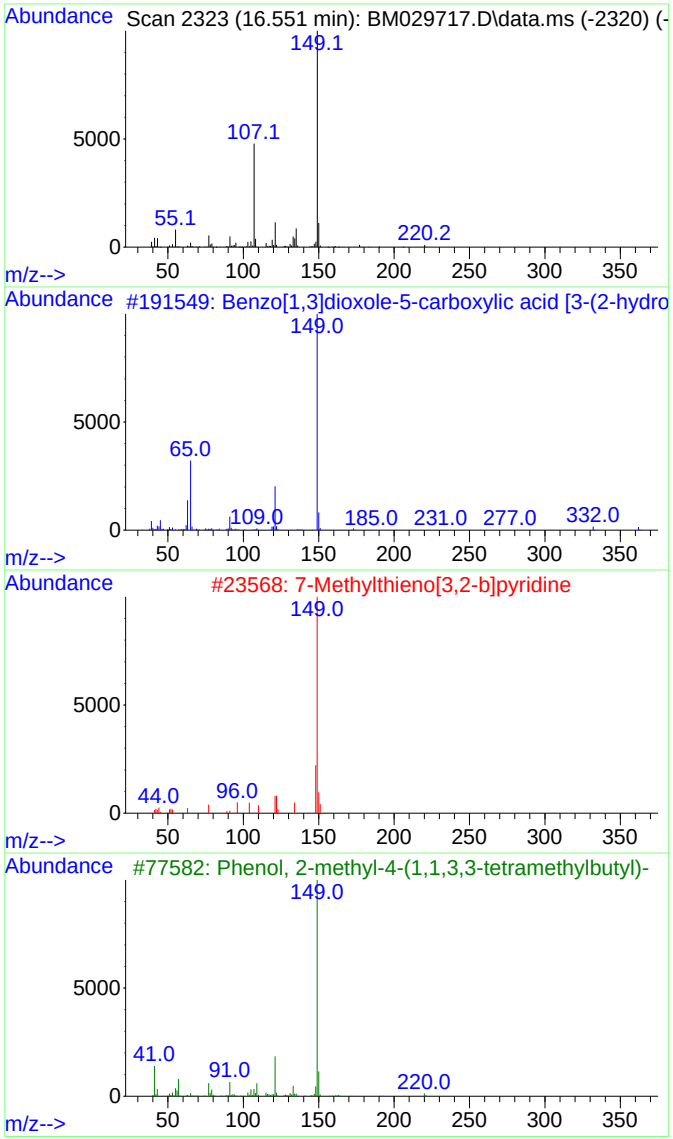
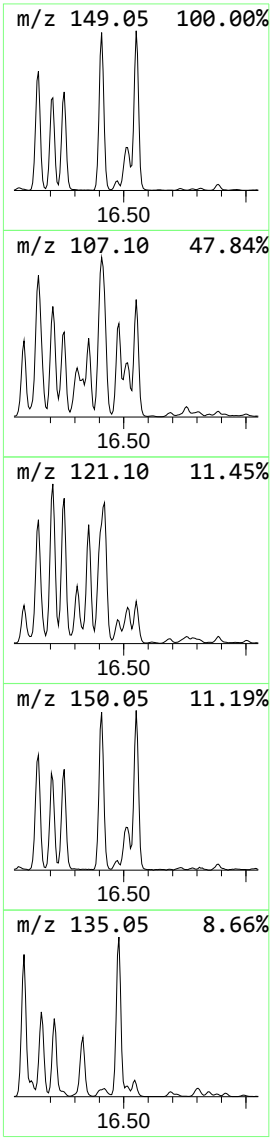
Peak Number 14 unknown16.551 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	41.83 ng	2054450	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[1,3]dioxole-5-carboxylic a...	362	C16H14N2O6S	1000296-89-7	47
2	7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	47
3	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	47
4	3-Ethoxy-4-hydroxyphenylacetonit...	177	C10H11NO2	205748-01-2	43
5	Benzene, 1-isocyanato-4-methoxy-	149	C8H7NO2	005416-93-3	40





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Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId :
SAMPLE-1-GRAB

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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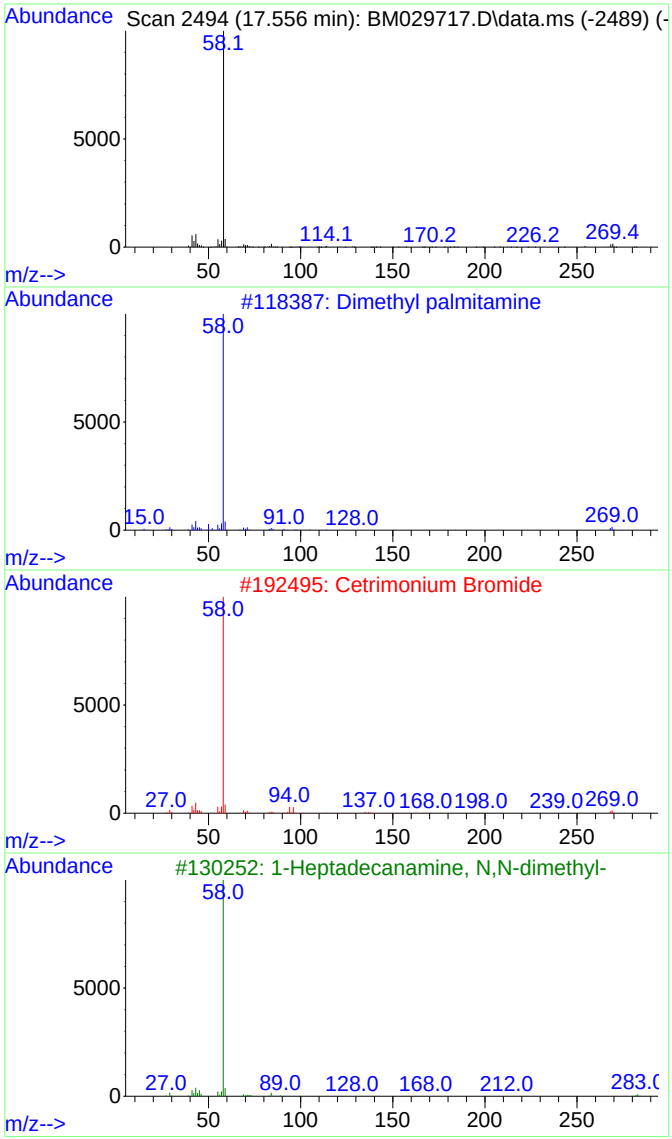
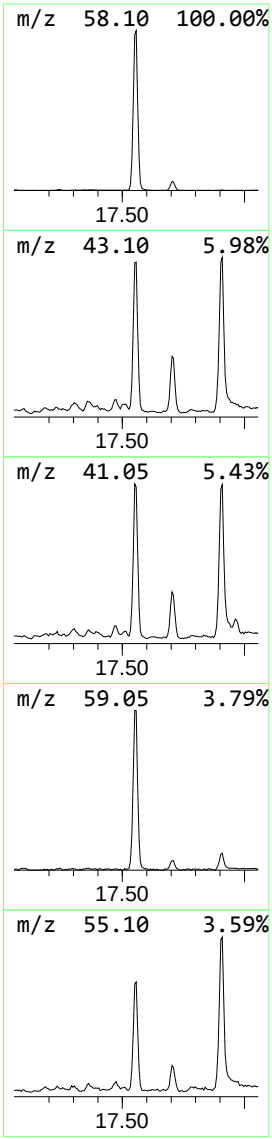
Peak Number 15 Cetrimonium Bromide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.556	30.62 ng	1504090	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl palmitamine	269	C18H39N	000112-69-6	91
2	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	78
3	1-Heptadecanamine, N,N-dimethyl-	283	C19H41N	003002-57-1	72
4	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	72
5	Tetradonium Bromide	335	C17H38BrN	001119-97-7	72





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ALS Vial : 14 Sample Multiplier: 1

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ClientSampleId :
SAMPLE-1-GRAB

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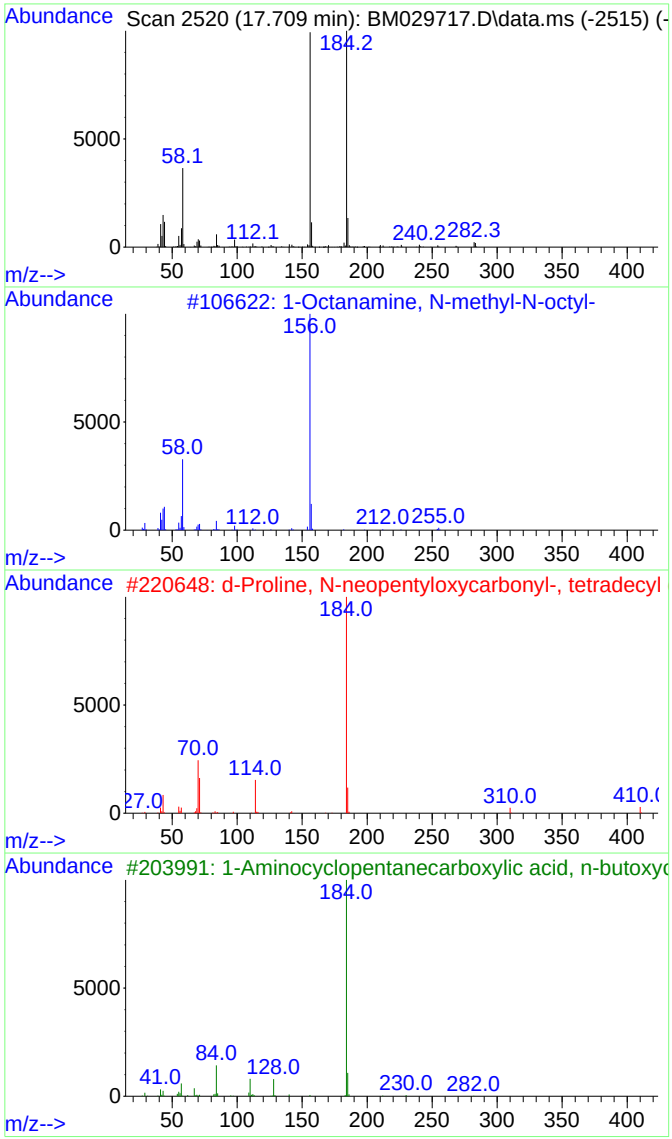
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

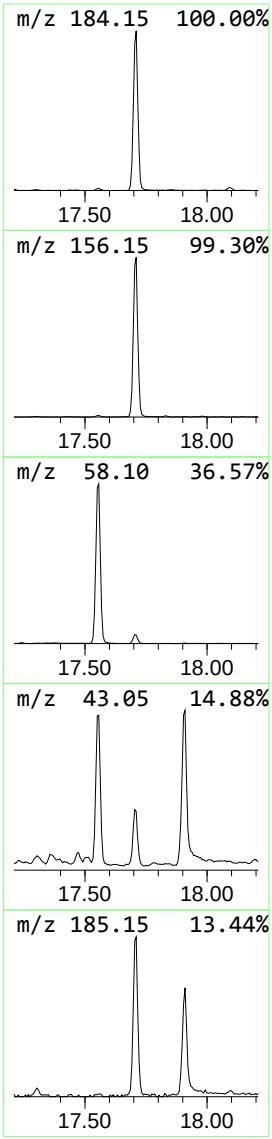
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 unknown17.709 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	11.99 ng	588753	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanamine, N-methyl-N-octyl-	255	C17H37N	004455-26-9	46
2	d-Proline, N-neopentyloxycarbony...	425	C25H47NO4	1000328-21-4	27
3	1-Aminocyclopentanecarboxylic ac...	383	C22H41NO4	1000329-09-6	27
4	1-Aminocyclopentanecarboxylic ac...	425	C25H47NO4	1000329-09-8	27
5	1-Aminocyclopentanecarboxylic ac...	313	C17H31NO4	1000329-10-2	27





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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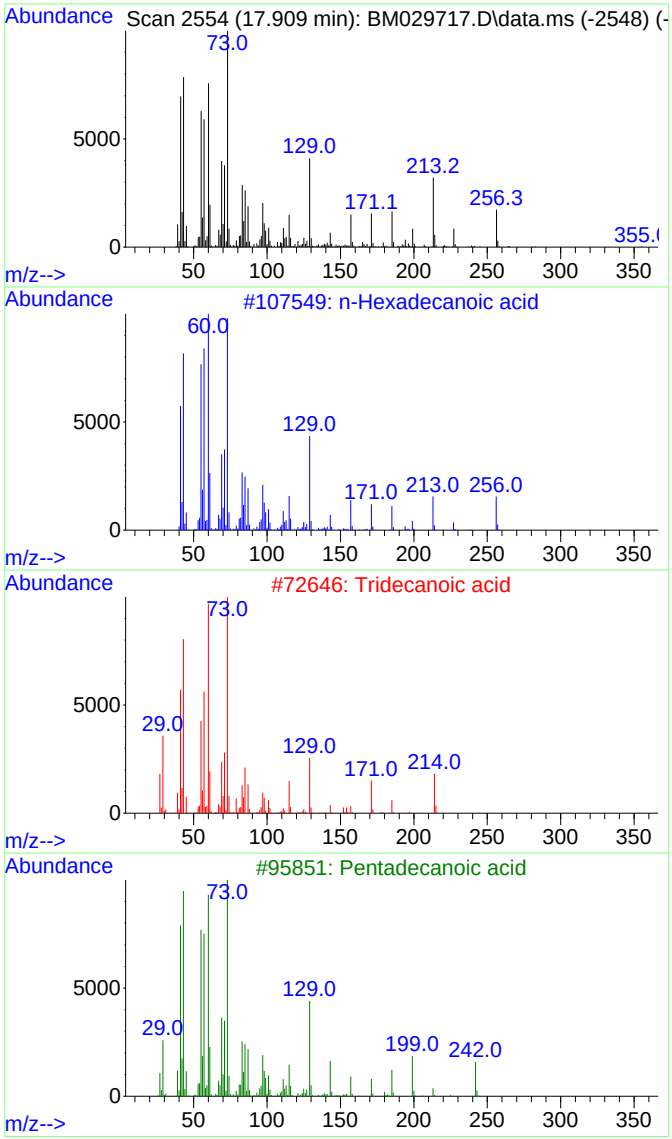
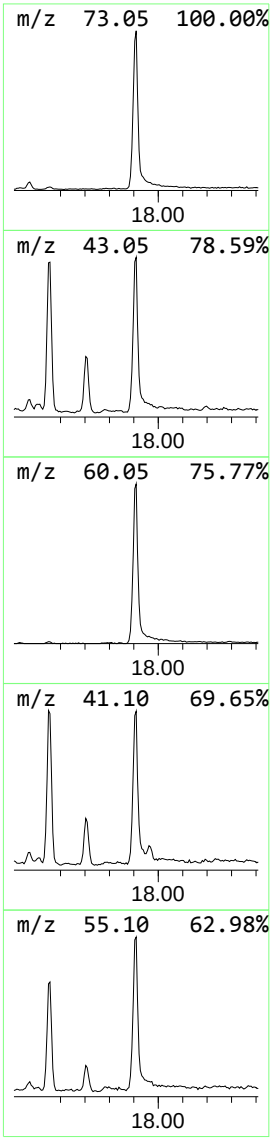
Peak Number 17 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.909	21.72 ng	1066580	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81





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Data File : BM029717.D
Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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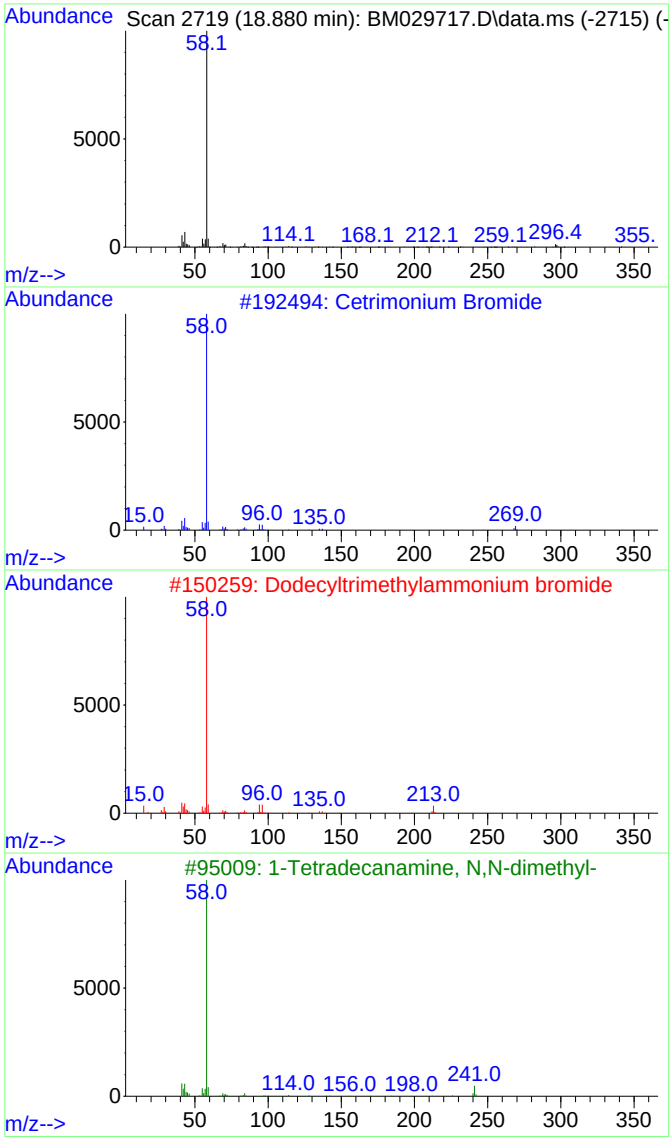
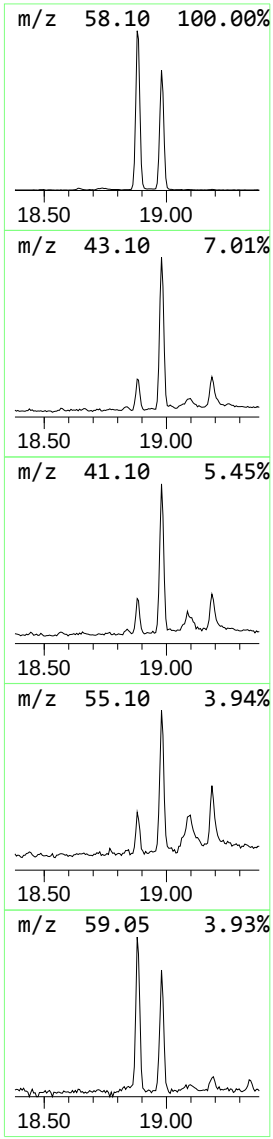
Peak Number 18 Dodecyltrimethylammonium br... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.880	6.38 ng	313310	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetrimonium Bromide	363	C19H42BrN	000057-09-0	78
2	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	78
3	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	78
4	3(N,N-Dimethylmyristylammonio)pr...	363	C19H41NO3S	014933-09-6	78
5	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	78





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Data File : BM029717.D
Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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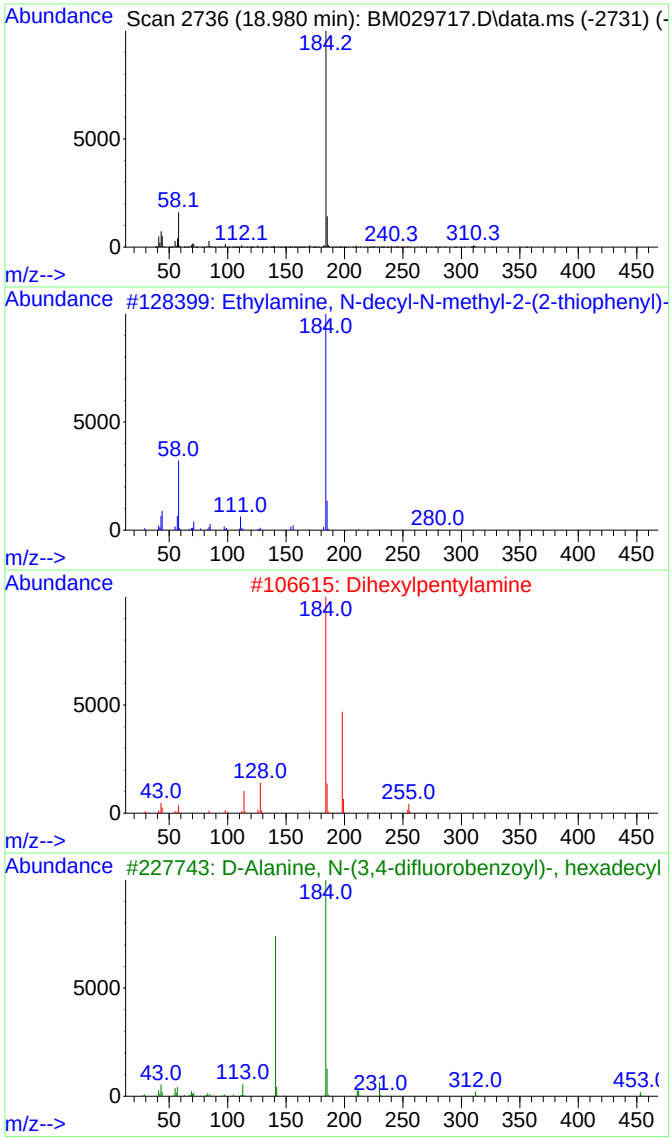
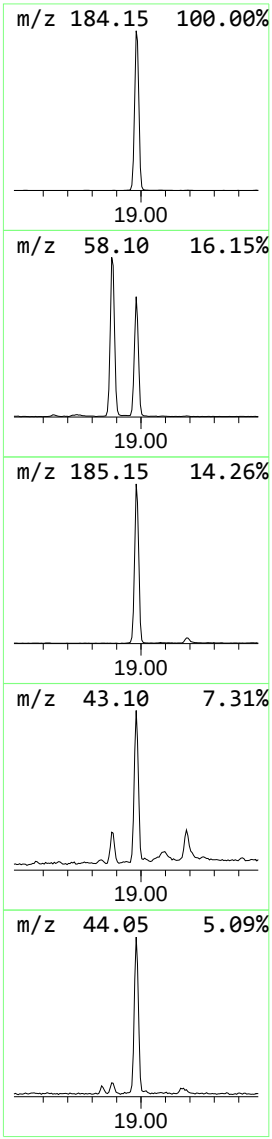
Peak Number 19 Ethylamine, N-decyl-N-methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.980	37.06 ng	1820140	Phenanthrene-d10	16.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylamine, N-decyl-N-methyl-2-(...	281	C17H31NS	1000310-34-4	72
2	Dihexylpentylamine	255	C17H37N	1000310-30-3	64
3	D-Alanine, N-(3,4-difluorobenzoy...	453	C26H41F2NO3	1000348-37-1	59
4	D-Alanine, N-(2,6-difluorobenzoy...	453	C26H41F2NO3	1000354-11-2	59
5	1-Aminocyclopentanecarboxylic ac...	313	C17H31NO4	1000329-09-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SAMPLE-1-GRAB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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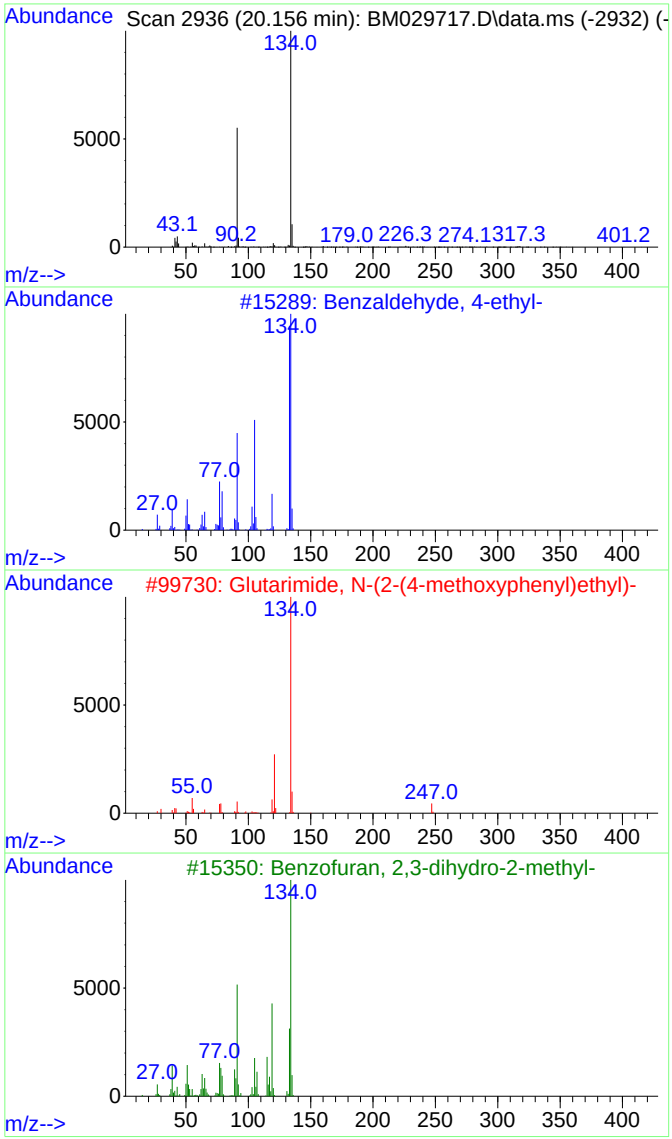
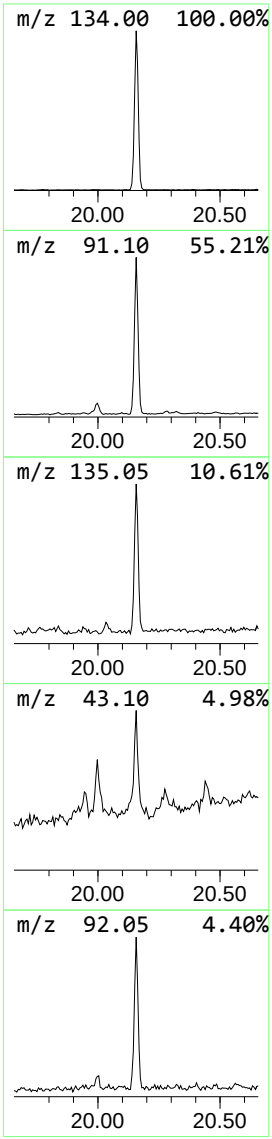
Peak Number 20 Benzaldehyde, 4-ethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.156	6.83 ng	382438	Chrysene-d12	21.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-ethyl-	134	C9H10O	004748-78-1	78
2	Glutarimide, N-(2-(4-methoxyphen...	247	C14H17NO3	1000360-22-8	50
3	Benzofuran, 2,3-dihydro-2-methyl-	134	C9H10O	001746-11-8	50
4	N-Methyl-N-benzyltetradecanamine	317	C22H39N	083690-72-6	46
5	Benzene, 1-ethenyl-4-methoxy-	134	C9H10O	000637-69-4	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM043021\
Data File : BM029717.D
Acq On : 29 Apr 2021 19:59
Operator : CG/JU
Sample : M2198-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SAMPLE-1-GRAB

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM043021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,4,6-Trimethyl...	11.827	7.5	ng	241763	2	10.374	645421	20.0
1-Decanamine, N...	11.880	9.1	ng	292651	2	10.374	645421	20.0
2-Acetamidotropone	15.998	31.0	ng	1523800	4	16.992	982324	20.0
Dimethyl palmit...	16.033	62.5	ng	3072000	4	16.992	982324	20.0
Phenol, 4-(1,1,...	16.092	61.9	ng	3041680	4	16.992	982324	20.0
unknown16.151	16.151	88.1	ng	4328360	4	16.992	982324	20.0
Phenol, p-tert-...	16.209	69.8	ng	3427070	4	16.992	982324	20.0
Phenol, 2-(1,1-...	16.256	41.7	ng	2046330	4	16.992	982324	20.0
Phenol, 4-(1,1-...	16.333	44.0	ng	2162690	4	16.992	982324	20.0
Acetamide, N-(2...	16.357	22.8	ng	1119050	4	16.992	982324	20.0
2-Methyl-4-hydr...	16.409	83.7	ng	4112470	4	16.992	982324	20.0
4-(1,1-Dimethyl...	16.480	70.1	ng	3444770	4	16.992	982324	20.0
unknown16.515	16.515	24.1	ng	1186190	4	16.992	982324	20.0
unknown16.551	16.551	41.8	ng	2054450	4	16.992	982324	20.0
Cetrimonium Bro...	17.556	30.6	ng	1504090	4	16.992	982324	20.0
unknown17.709	17.709	12.0	ng	588753	4	16.992	982324	20.0
n-Hexadecanoic ...	17.909	21.7	ng	1066580	4	16.992	982324	20.0
Dodecyltrimethy...	18.880	6.4	ng	313310	4	16.992	982324	20.0
Ethylamine, N-d...	18.980	37.1	ng	1820140	4	16.992	982324	20.0
Benzaldehyde, 4...	20.156	6.8	ng	382438	5	21.174	1119760	20.0