LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

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-BM121621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.431	198	203	214	rVB	36365	56730	1.37%	0.128%
2	5.037	300	306	317	rBV	470065	676250	16.28%	1.524%
3	5.502	378	385	396	rBV	1281007	1851650	44.58%	4.174%
4	6.119	485	490	499	rBV	35785	52274	1.26%	0.118%
5	7.107	650	658	675	rBV	1257465	2077889	50.03%	4.684%
6	7.937	792	799	806	rBV	219658	367869	8.86%	0.829%
7	9.107	990	998	1009	rBV	818450	1386133	33.37%	3.125%
8	10.531	1233	1240	1252	rBV2	59582	124895	3.01%	0.282%
9	10.748	1269	1277	1283	rBV	285562	497539	11.98%	1.122%
10	13.089	1669	1675	1682	rVB2	35872	56982	1.37%	0.128%
11	13.207	1684	1695	1702	rBV	1987742	2905787	69.96%	6.550%
12	13.360	1716	1721	1726	rBV	174164	258220	6.22%	0.582%
13	13.483	1736	1742	1746	rBV3	65145	95100	2.29%	0.214%
14	13.589	1755	1760	1765	rVB2	60374	89393	2.15%	0.202%
15	13.760	1785	1789	1795	rVB4	28211	44652	1.08%	0.101%
16	13.848	1795	1804	1808	rBV	1636766	2368609	57.03%	5.340%
17	13.895	1808	1812	1817	rVB2	271183	429777	10.35%	0.969%
18	14.001	1823	1830	1834	rBV3	58233	106565	2.57%	0.240%
19	14.101	1841	1847	1854	rVB	146159	227968	5.49%	0.514%
20	14.225	1862	1868	1872	rBV4	28495	53119	1.28%	0.120%
21	14.307	1877	1882	1886	rVV	40996	59664	1.44%	0.135%
22	14.395	1894	1897	1903	rVB4	53739	84973	2.05%	0.192%
23	14.472	1903	1910	1915	rVB2	76010	127735	3.08%	0.288%
24	14.525	1915	1919	1923	rBV	21917	42750	1.03%	0.096%
25	14.583	1923	1929	1936	rVB	428526	676787	16.30%	1.526%
26	14.789	1958	1964	1967	rBV4	55798	106348	2.56%	0.240%
27	14.830	1967	1971	1979	rVB	171447	283828	6.83%	0.640%
28	15.013	1992	2002	2008	rBV	97484	179189	4.31%	0.404%
29	15.366	2055	2062	2066	rBV4	26367	50705	1.22%	0.114%
30	15.748	2119	2127	2131	rBV7	22143	43380	1.04%	0.098%
31	15.813	2132	2138	2142	rVV2	120207	202060	4.87%	0.456%
32	15.866	2142	2147	2155	rVB	876332	1262774	30.40%	2.847%
33	16.071	2176	2182	2188	rBV	1508056	2150024	51.77%	4.847%
34	16.177	2196	2200	2208	rVB2	62592	88128	2.12%	0.199%
35	16.307	2215	2222	2228	rBV4	65616	155594	3.75%	0.351%
36	16.601	2261	2272	2284	rBV9	63456	182648	4.40%	0.412%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

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-BM121621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.719	2289	2292	2298	rVB8	26532	47688	1.15%	0.108%
38	17.077	2347	2353	2359	rBV8	28871	62277	1.50%	0.140%
39	17.242	2377	2381	2385	rVB	45321	56426	1.36%	0.127%
40	17.330	2390	2396	2401	rBV	506120	734107	17.68%	1.655%
41	17.460	2414	2418	2423	rBV	46135	63420	1.53%	0.143%
42	17.613	2439	2444	2447	rBV	51199	84338	2.03%	0.190%
43	17.995	2505	2509	2514	rVB	79729	107466	2.59%	0.242%
44	18.218	2542	2547	2551	rBV2	157300	239294	5.76%	0.539%
45	18.295	2557	2560	2564	rVB	67187	78554	1.89%	0.177%
46	18.401	2573	2578	2583	rBV4	81176	164004	3.95%	0.370%
47	18.518	2594	2598	2602	rBV5	42520	60076	1.45%	0.135%
48	19.124	2696	2701	2705	rBV	125181	224970	5.42%	0.507%
49	19.183	2706	2711	2715	rVB3	102796	180226	4.34%	0.406%
50	19.265	2720	2725	2731	rBV3	103425	228976	5.51%	0.516%
51	19.383	2740	2745	2750	rBV	301749	413328	9.95%	0.932%
52	19.495	2760	2764	2769	rBV5	49932	70004	1.69%	0.158%
53	19.748	2799	2807	2815	rBV	799986	1222034	29.42%	2.755%
54	19.818	2815	2819	2825	rVB2	81107	142103	3.42%	0.320%
55	19.954	2836	2842	2852	rVB	2823059	3636681	87.56%	8.198%
56	20.071	2858	2862	2871	rVB3	139301	332799	8.01%	0.750%
57	20.224	2881	2888	2896	rVB3	199438	554482	13.35%	1.250%
58	20.342	2905	2908	2913	rBV2	78611	111089	2.67%	0.250%
59	20.401	2914	2918	2920	rVV2	238078	356449	8.58%	0.804%
60	20.436	2920	2924	2935	rVB3	474123	817490	19.68%	1.843%
61	20.542	2938	2942	2945	rBV	285162	368309	8.87%	0.830%
62	20.595	2945	2951	2955	rVV2	3243304	4153314	100.00%	9.363%
63	20.636	2955	2958	2964	rVB	831251	1137935	27.40%	2.565%
64	20.830	2988	2991	2994	rBV4	66040	87124	2.10%	0.196%
65	21.212	3050	3056	3062	rBV3	151484	388224	9.35%	0.875%
66	21.259	3062	3064	3067	rVV3	64401	68916	1.66%	0.155%
67	21.418	3086	3091	3098	rVB	2160453	2326038	56.00%	5.244%
68	21.501	3099	3105	3110	rBV2	535856	1249370	30.08%	2.816%
69	21.548	3110	3113	3119	rVB	411607	563268	13.56%	1.270%
70	21.671	3131	3134	3141	rBV3	85442	220452	5.31%	0.497%
71	22.089	3201	3205	3209	rVV	225456	318386	7.67%	0.718%
72	22.142	3209	3214	3221	rVB2	734323	1125636	27.10%	2.538%
73	22.301	3238	3241	3244	rBV3	111886	132897	3.20%	0.300%
74	22.759	3316	3319	3330	rVB2	184802	362741	8.73%	0.818%
75	23.189	3387	3392	3405	rVB2	276739	883143	21.26%	1.991%
76	23.712	3477	3481	3490	rVB	241538	489230	11.78%	1.103%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

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-BM121621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	23.818	3494	3499	3506	rVB	383989	757373	18.24%	1.707%
78	23.924	3513	3517	3523	rVB2	177101	315175	7.59%	0.710%

Sum of corrected areas: 44359800

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
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Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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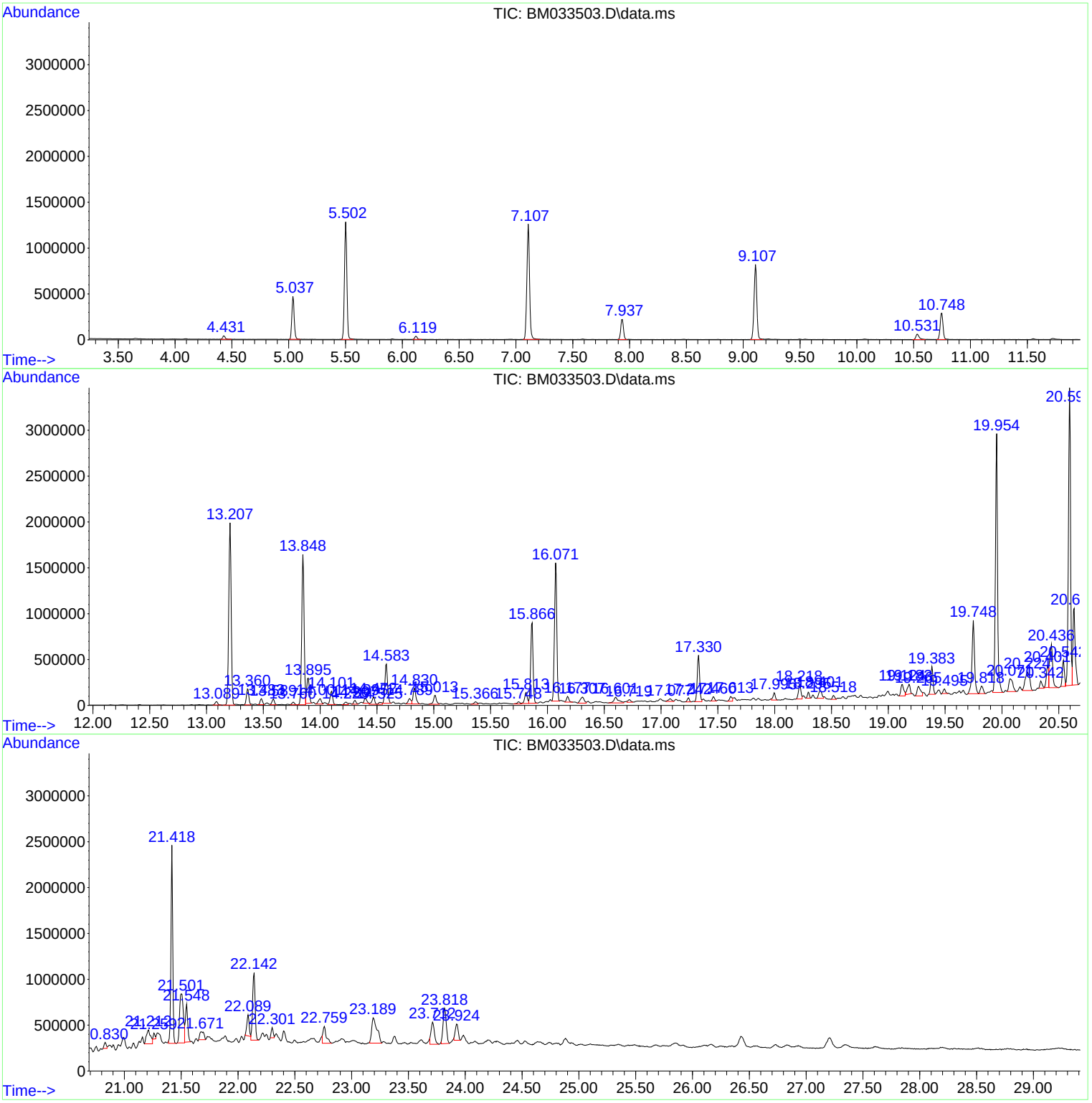
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

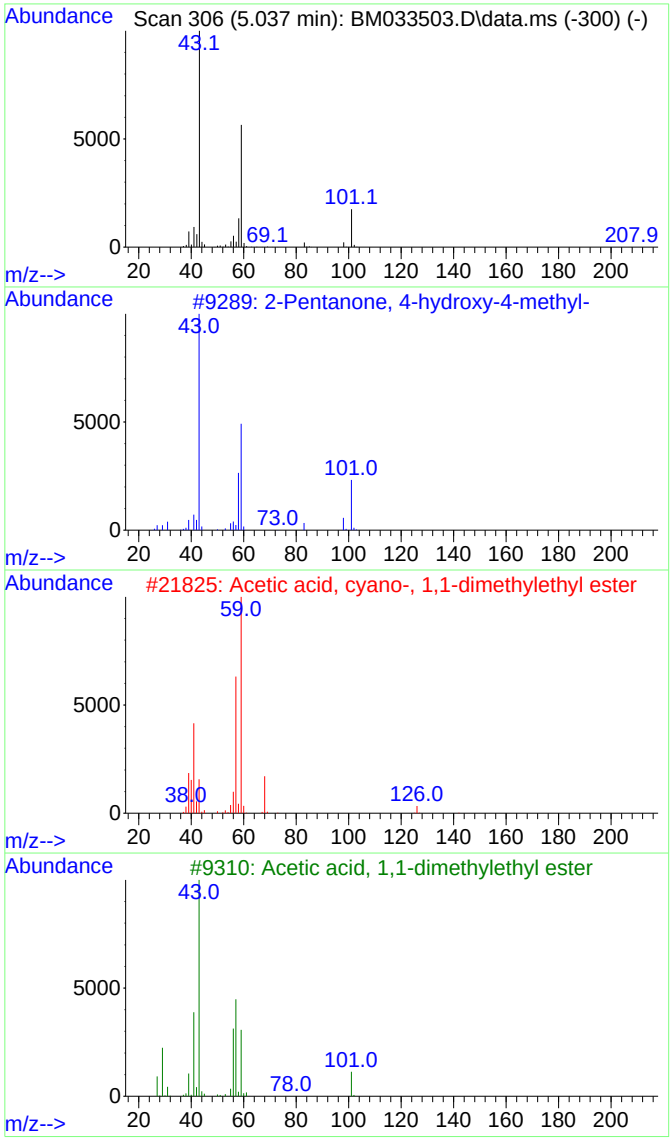
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

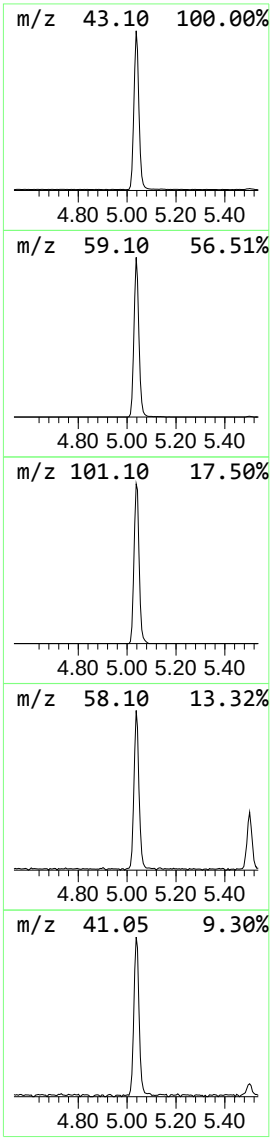
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.037	36.77 ng	676250	1,4-Dichlorobenzene-d4	7.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

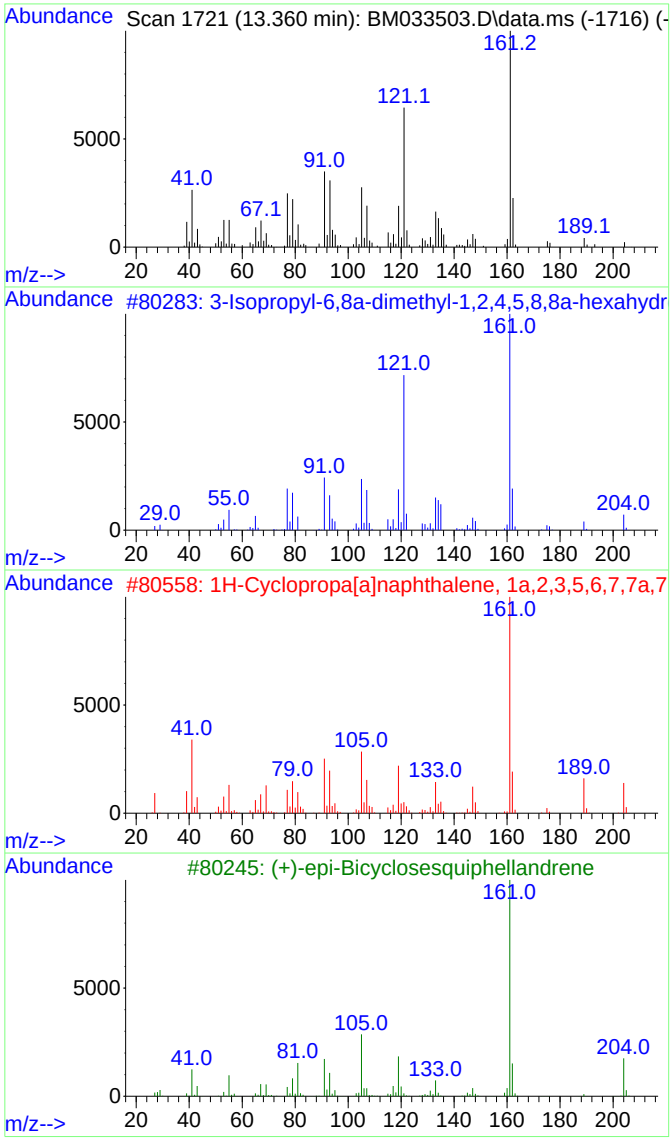
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

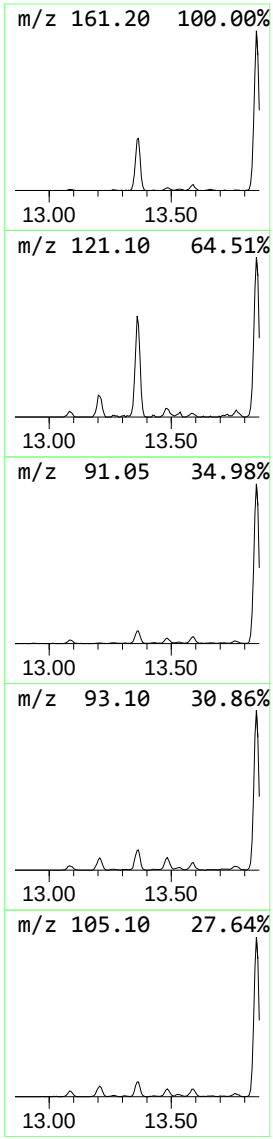
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Isopropyl-6,8a-dimethyl-1... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.360	7.63 ng	258220	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Isopropyl-6,8a-dimethyl-1,2,4,...	204	C15H24	016661-00-0	81
2	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	76
3	(+)-epi-Bicyclosesquiphellandrene	204	C15H24	054274-73-6	60
4	cis-Muurola-4(15),5-diene	204	C15H24	157477-72-0	49
5	1H-1,2,4-Triazol-3-amine, 5-(4-p...	161	C7H7N5	003652-17-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

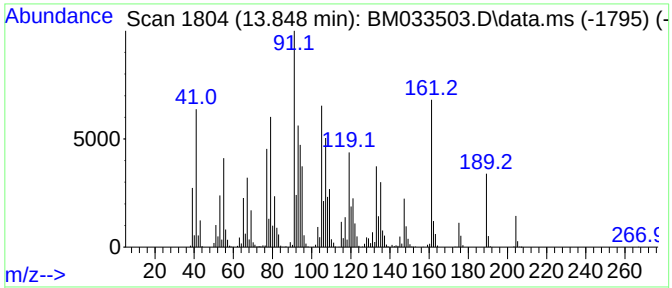
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

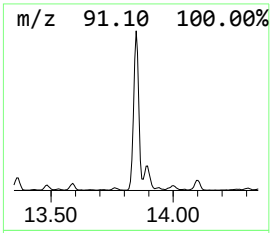
****

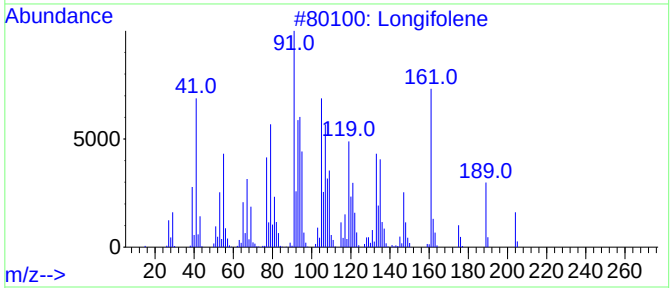
Peak Number 3 Longifolene Concentration Rank 1

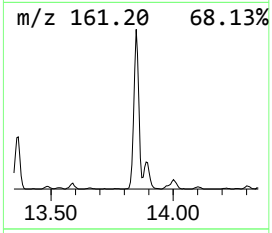
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.848	70.00 ng	2368610	Acenaphthene-d10	14.583

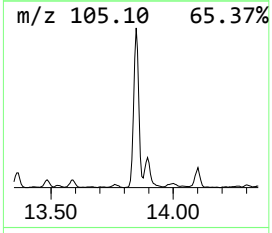
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Longifolene	204	C15H24	000475-20-7	99
2	Aromandendrene	204	C15H24	000489-39-4	91
3	(4S,4aR,6R)-4,4a-Dimethyl-6-(pro...	204	C15H24	054868-40-5	89
4	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	83
5	Germacrene D	204	C15H24	023986-74-5	72

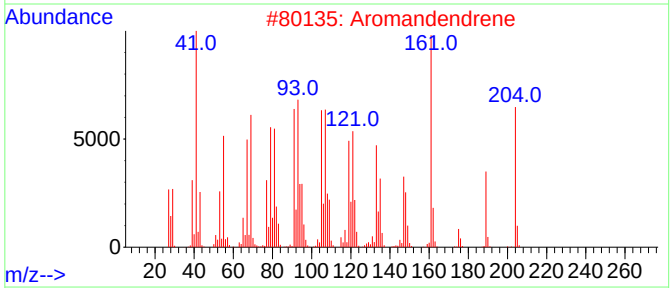


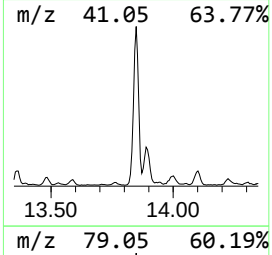


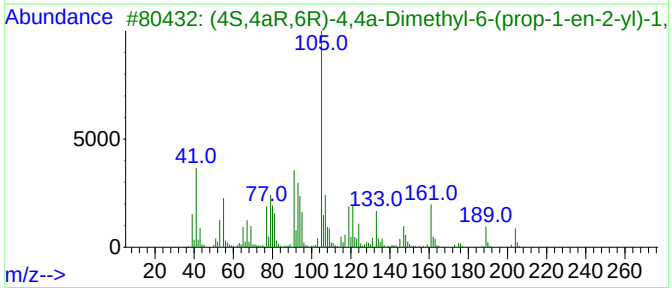


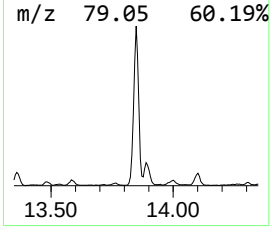












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
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Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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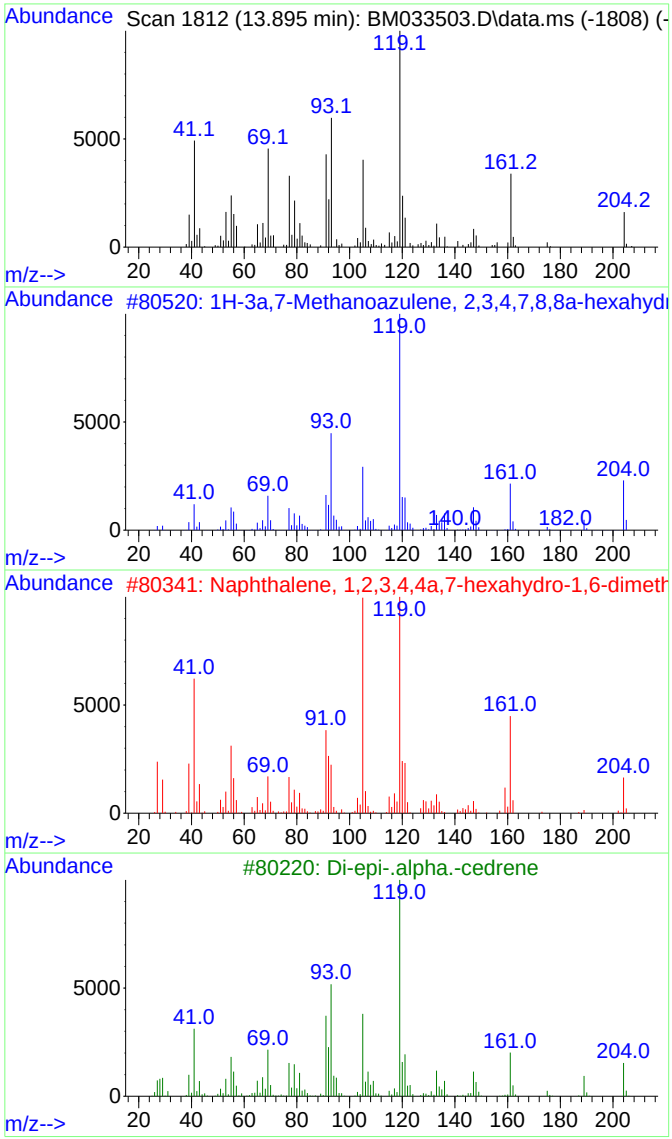
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

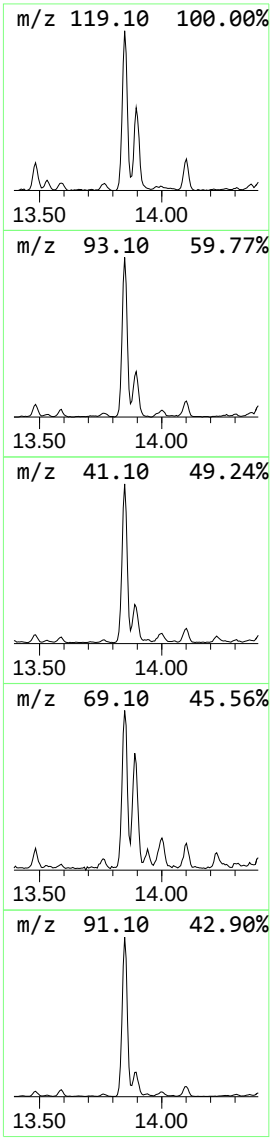
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.895	12.70 ng	429777	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	76
2	Naphthalene, 1,2,3,4,4a,7-hexahy...	204	C15H24	016728-99-7	58
3	Di-epi-.alpha.-cedrene	204	C15H24	050894-66-1	58
4	Tricyclo[5.4.0.0(2,8)]undec-9-en...	204	C15H24	005989-08-2	49
5	Di-epi-.alpha.-cedrene-(I)	204	C15H24	021996-77-0	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

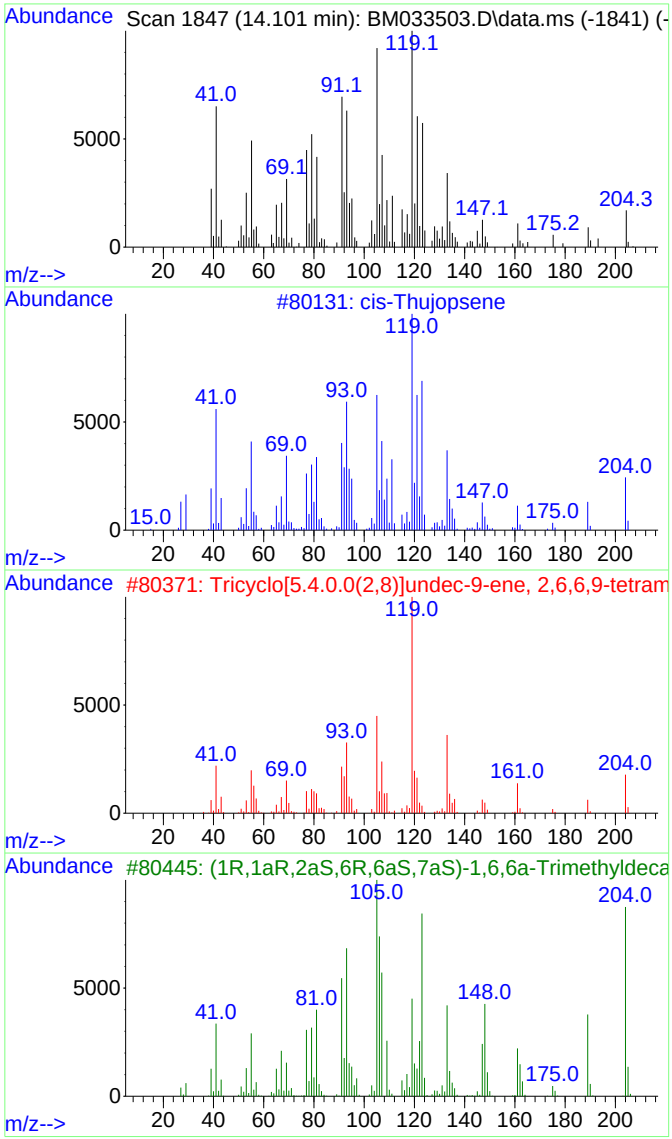
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

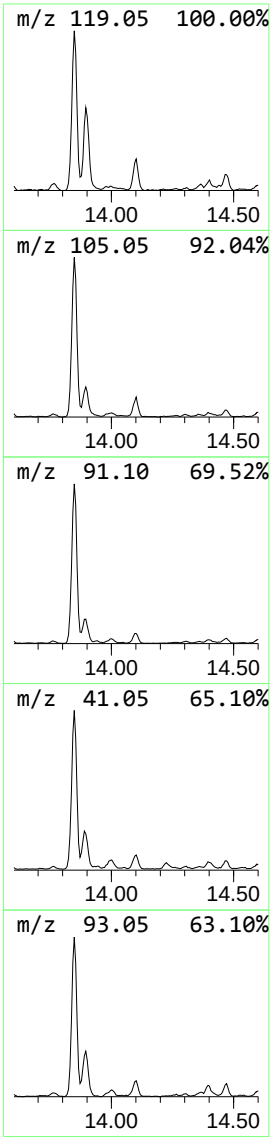
****

Peak Number 5 cis-Thujopsene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.101	6.74 ng	227968	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Thujopsene	204	C15H24	000470-40-6	99
2	Tricyclo[5.4.0.0(2,8)]undec-9-en...	204	C15H24	005989-08-2	83
3	(1R,1aR,2aS,6R,6aS,7aS)-1,6,6a-T...	204	C15H24	026620-70-2	66
4	7-epi-Silphiperfol-5-ene	204	C15H24	138752-23-5	64
5	(Z,Z)-.alpha.-Farnesene	204	C15H24	1000293-03-1	50





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Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

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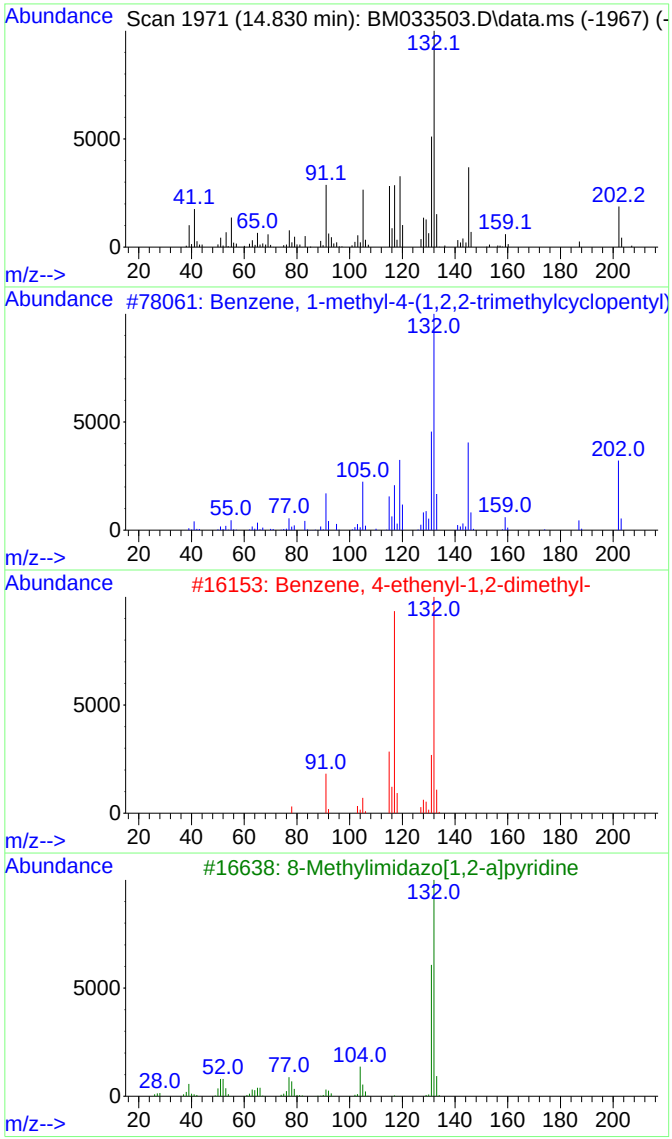
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

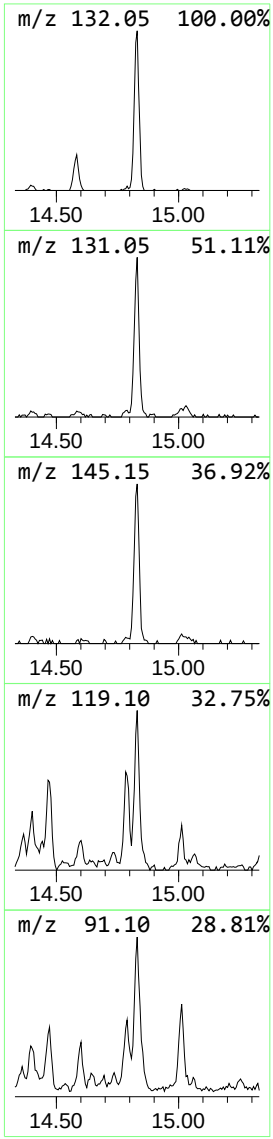
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-methyl-4-(1,2,2-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.830	8.39 ng	283828	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(1,2,2-trime...	202	C15H22	016982-00-6	97
2	Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	027831-13-6	47
3	8-Methylimidazo[1,2-a]pyridine	132	C8H8N2	000874-10-2	46
4	5-Methylimidazo[1,2-a]pyridine	132	C8H8N2	000933-69-7	43
5	1-Methylbenzimidazole	132	C8H8N2	001632-83-3	43





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ClientSampleId :
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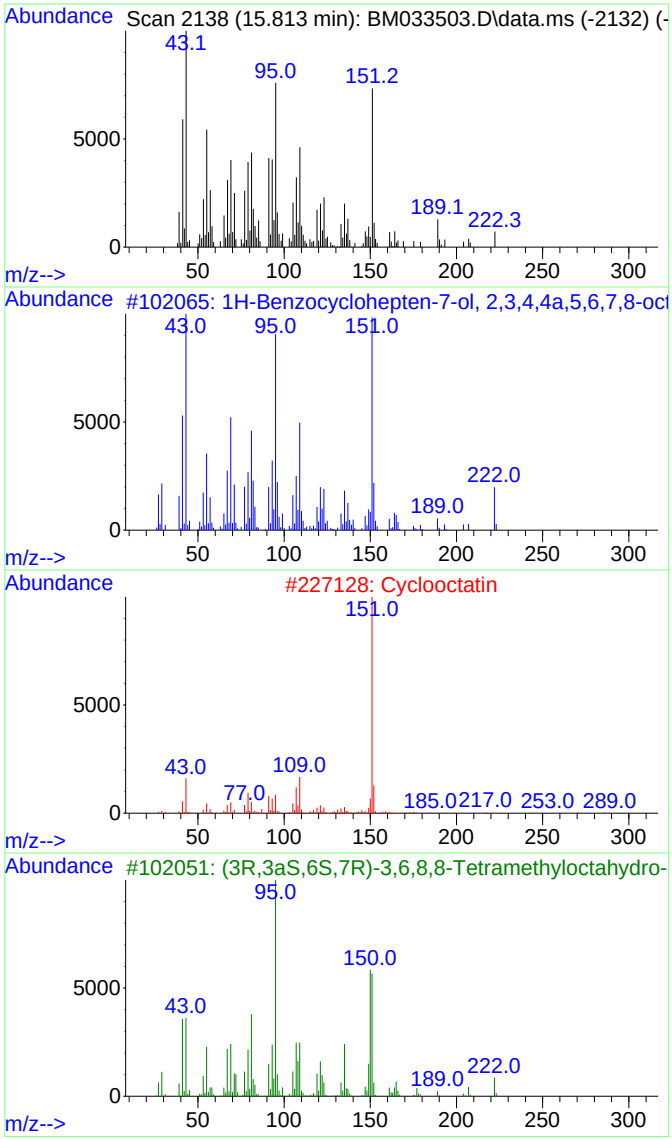
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

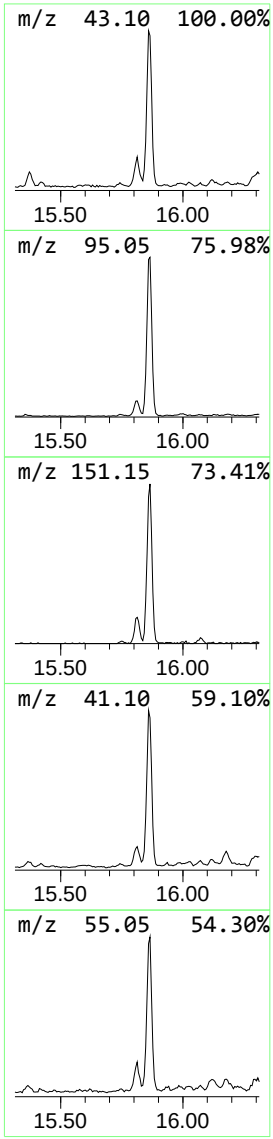
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Benzocyclohepten-7-ol, 2... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.813	5.97 ng	202060	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzocyclohepten-7-ol, 2,3,4,...	222	C15H26O	006892-80-4	93
2	Cyclooctatin	322	C20H34O3	139552-97-9	47
3	(3R,3aS,6S,7R)-3,6,8,8-Tetrameth...	222	C15H26O	019903-73-2	38
4	(3E,5E)-2,6-Dimethylocta-3,5,7-t...	152	C10H16O	206115-88-0	35
5	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	35





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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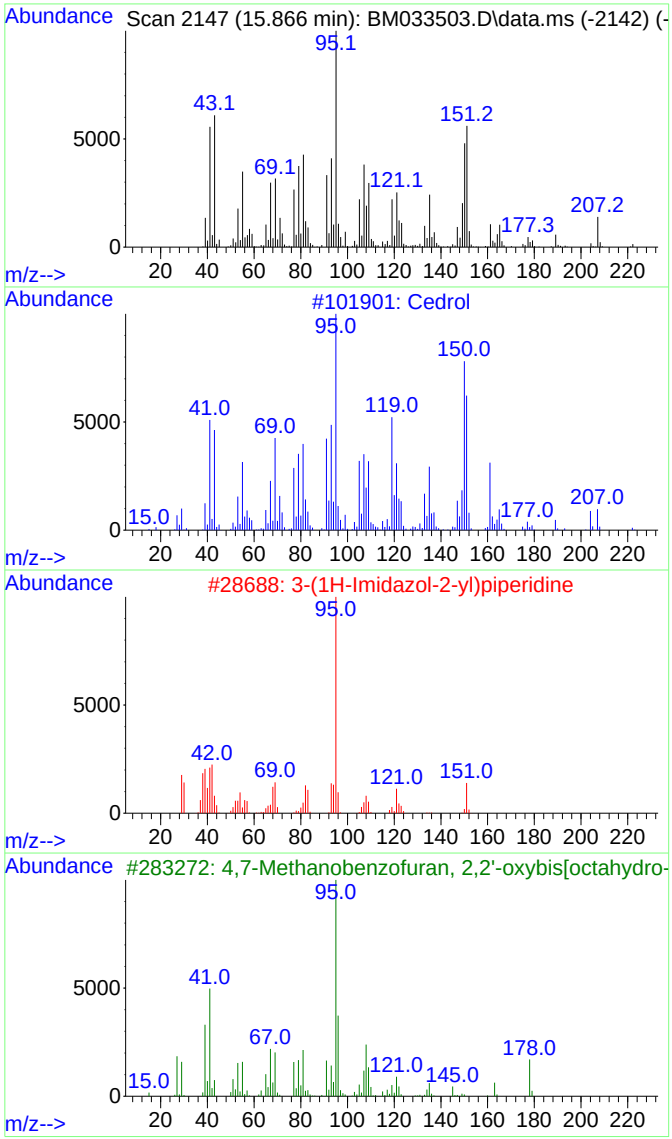
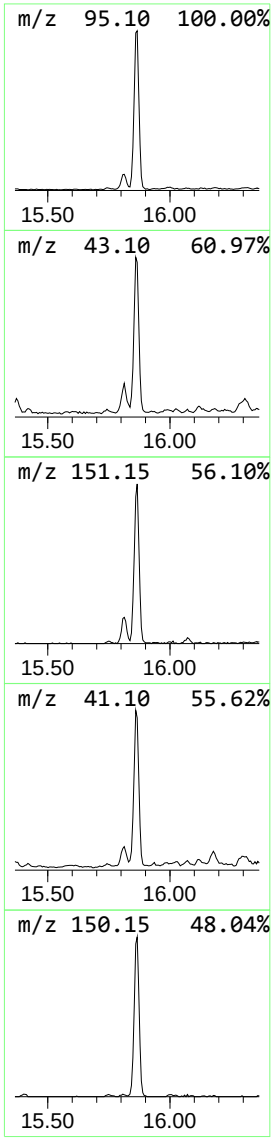
Peak Number 8 Cedrol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.866	37.32 ng	1262770	Acenaphthene-d10	14.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cedrol	222	C15H26O	000077-53-2	90
2	3-(1H-Imidazol-2-yl)piperidine	151	C8H13N3	1000444-58-0	35
3	4,7-Methanobenzofuran, 2,2'-oxyb...	374	C24H38O3	087248-50-8	27
4	Ethanethioamide, N-phenyl-	151	C8H9NS	000637-53-6	25
5	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	22





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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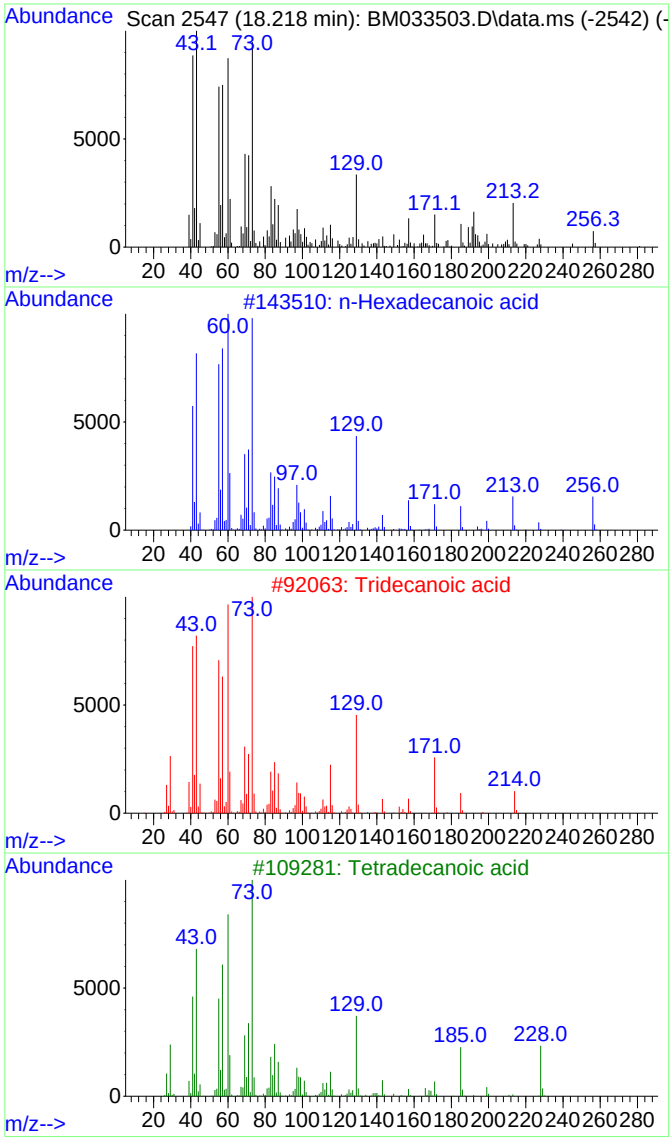
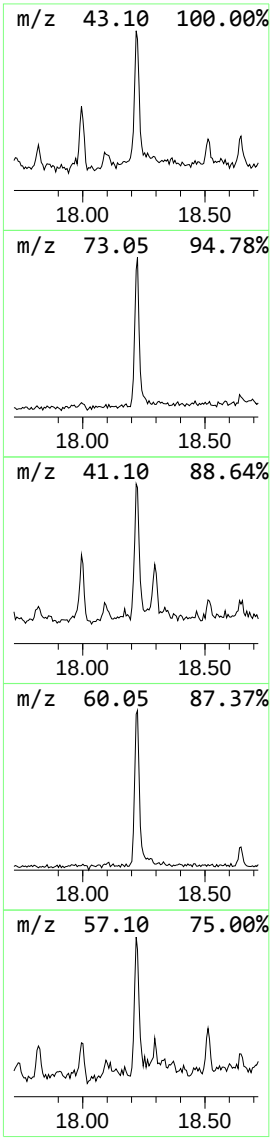
Peak Number 9 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	6.52 ng	239294	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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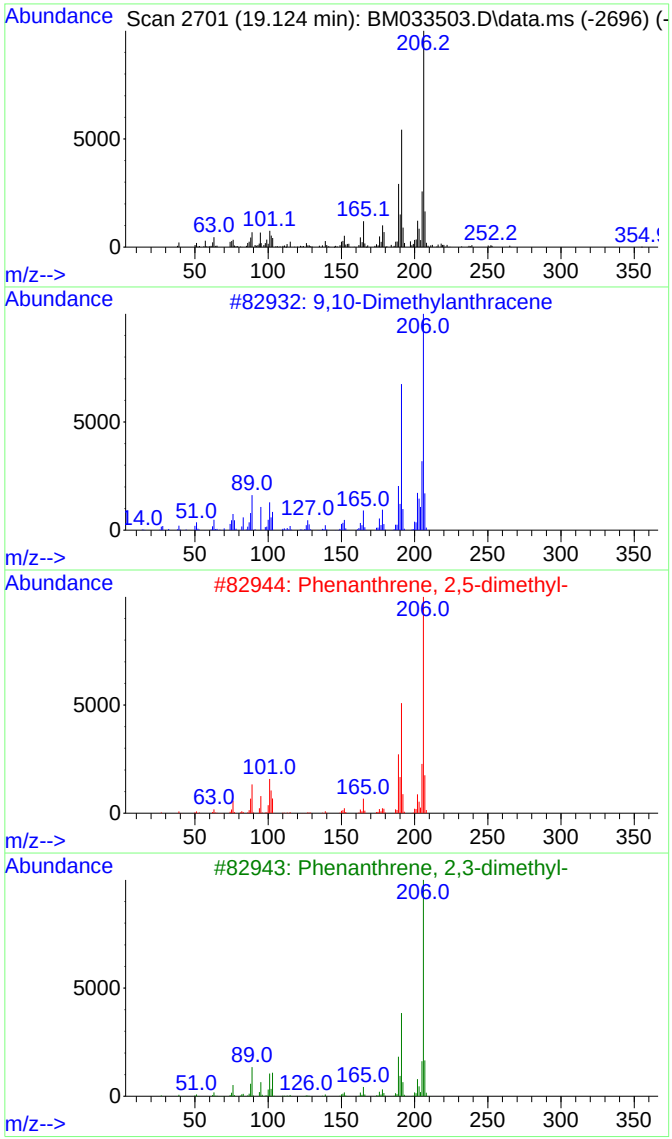
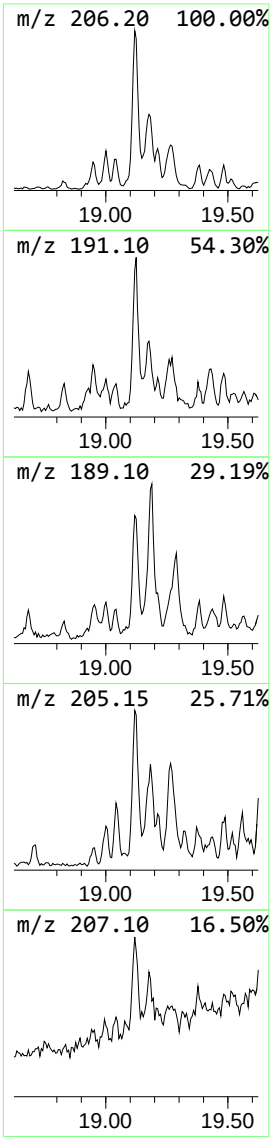
Peak Number 10 9,10-Dimethylanthracene Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.124	6.13 ng	224970	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
2	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
3	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	91
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	90
5	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	90





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Misc :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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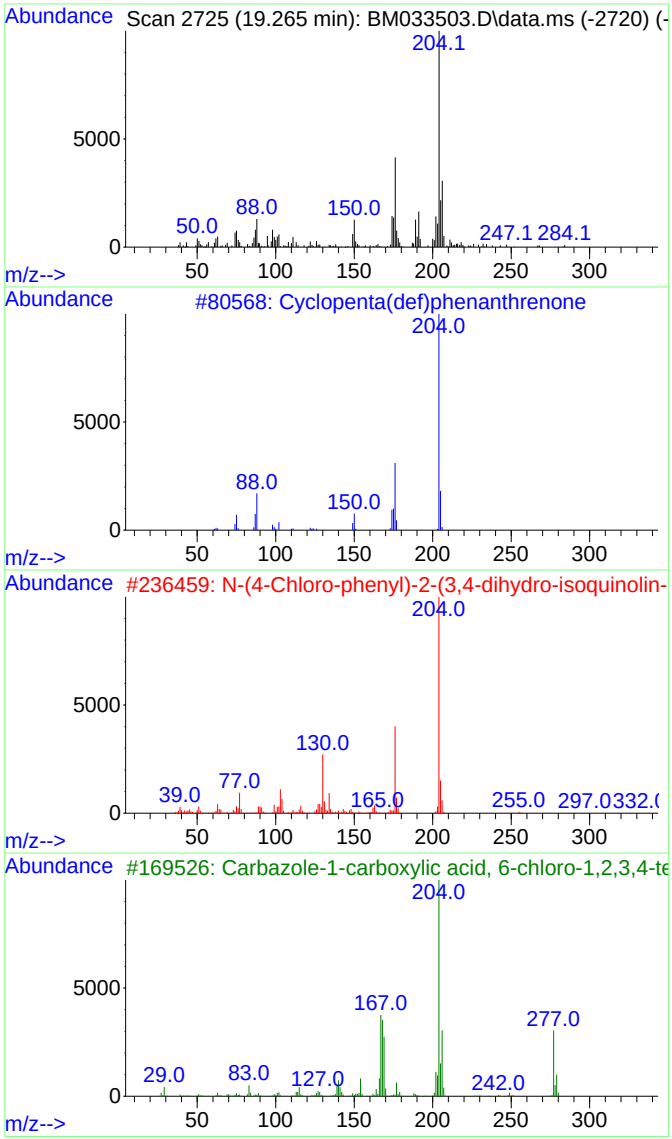
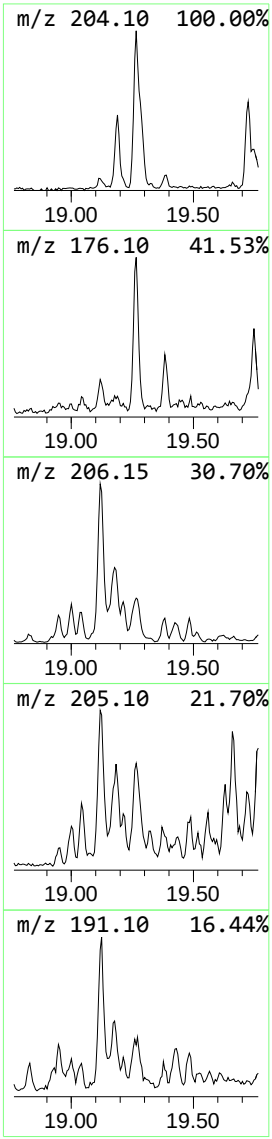
Peak Number 11 Cyclopenta(def)phenanthrenone Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.265	6.24 ng	228976	Phenanthrene-d10	17.330

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	70
2	N-(4-Chloro-phenyl)-2-(3,4-dihyd...	330	C17H15ClN2OS	1010296-34-3	53
3	Carbazole-1-carboxylic acid, 6-c...	277	C15H16ClNO2	049844-36-2	50
4	6-Chloro-2,3,4,9-tetrahydro-1H-c...	248	C13H13ClN2O	1000303-44-7	47
5	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	47





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Instrument :
BNA_M
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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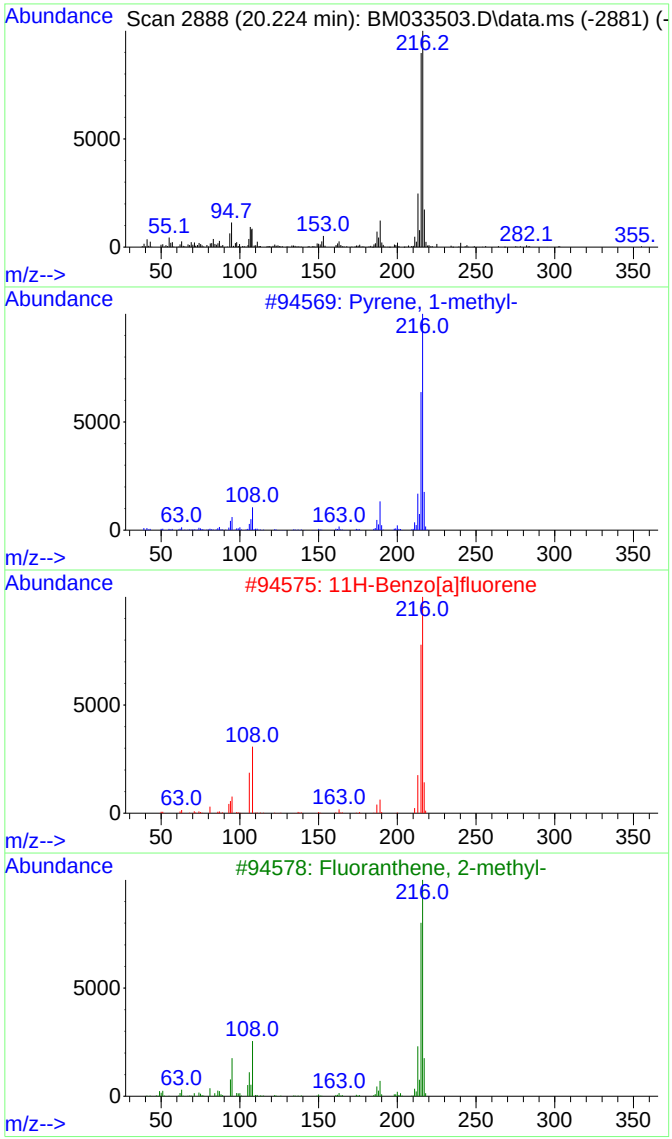
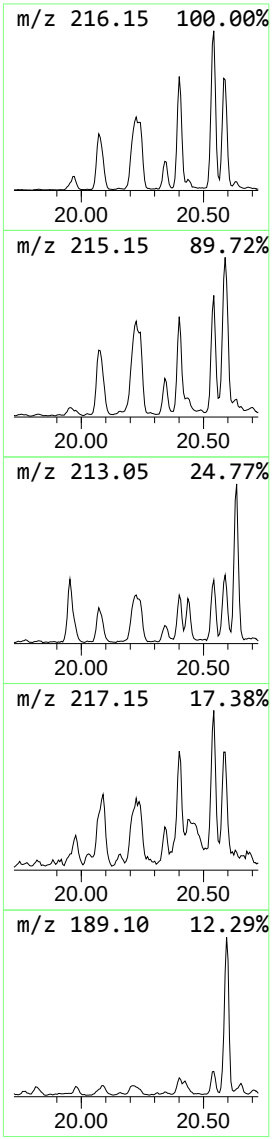
Peak Number 12 Pyrene, 1-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.224	8.88 ng	554482	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	87
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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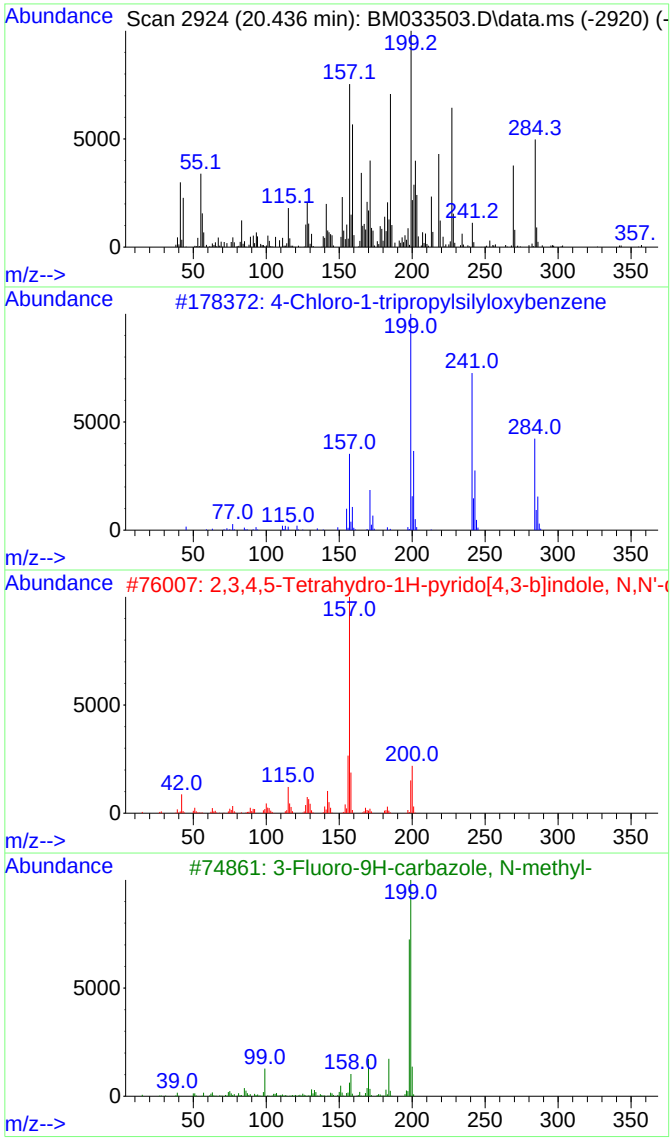
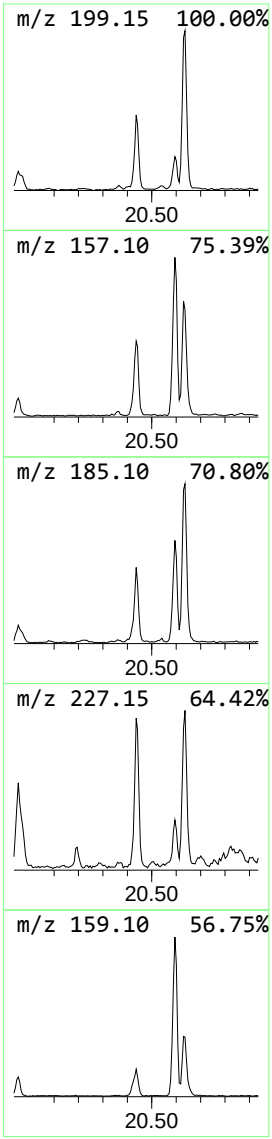
Peak Number 13 unknown20.436 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.436	13.09 ng	817490	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-1-tripropylsilyloxybenzene	284	C15H25ClOSi	1000307-84-1	25
2	2,3,4,5-Tetrahydro-1H-pyrido[4,3...	200	C13H16N2	003749-25-5	11
3	3-Fluoro-9H-carbazole, N-methyl-	199	C13H10FN	1440730-65-3	11
4	Androsta-5,7-diene, 4,4-dimethyl-	284	C21H32	1000194-15-2	11
5	2-(Diethylamino)-5,6-dimethylpyr...	228	C13H16N4	1000389-15-6	11





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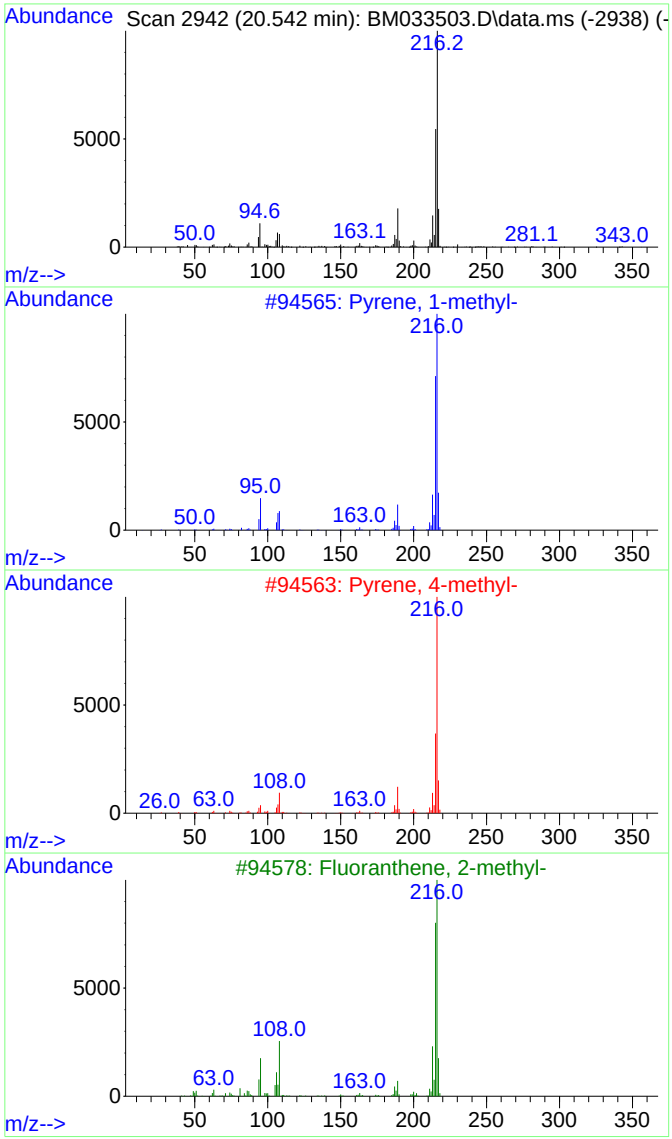
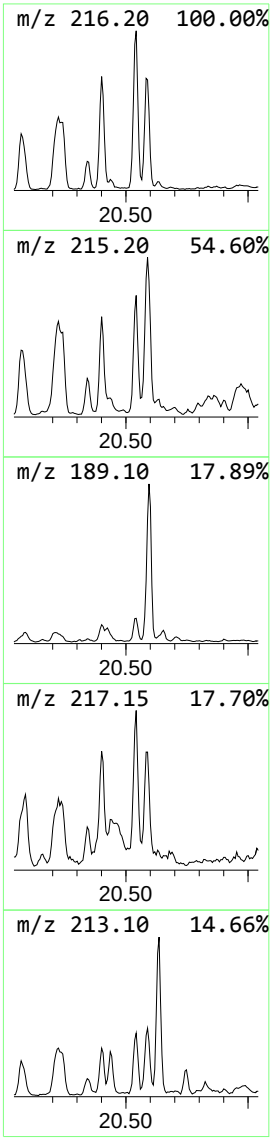
****

Peak Number 14 Pyrene, 4-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.542	5.90 ng	368309	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2	Pyrene, 4-methyl-	216	C17H12	003353-12-6	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	93
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90





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ClientSampleId :
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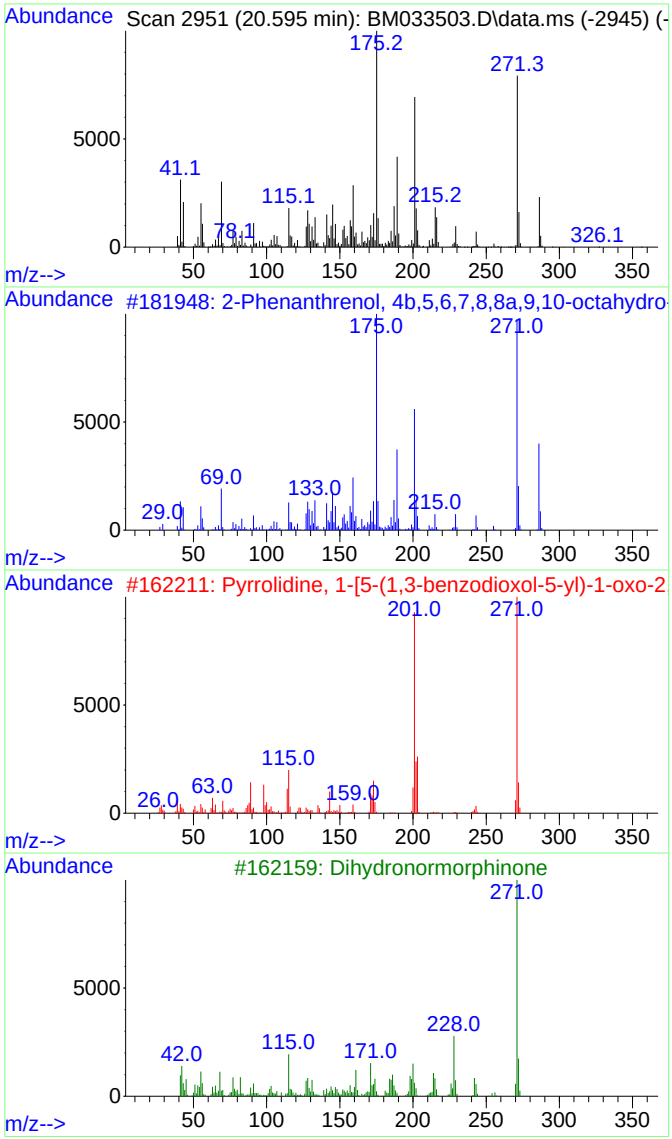
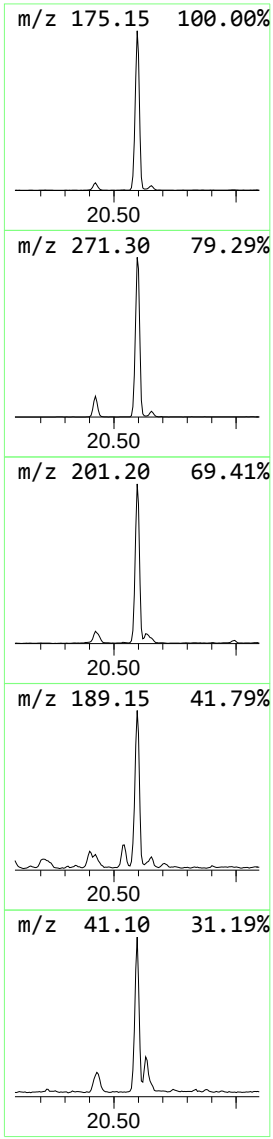
****
Peak Number 15 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.595	66.49 ng	4153310	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	38
3	Dihydronormorphinone	271	C16H17NO3	014696-23-2	25
4	Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	18
5	Crinan-1-one	271	C16H17NO3	098301-98-5	18





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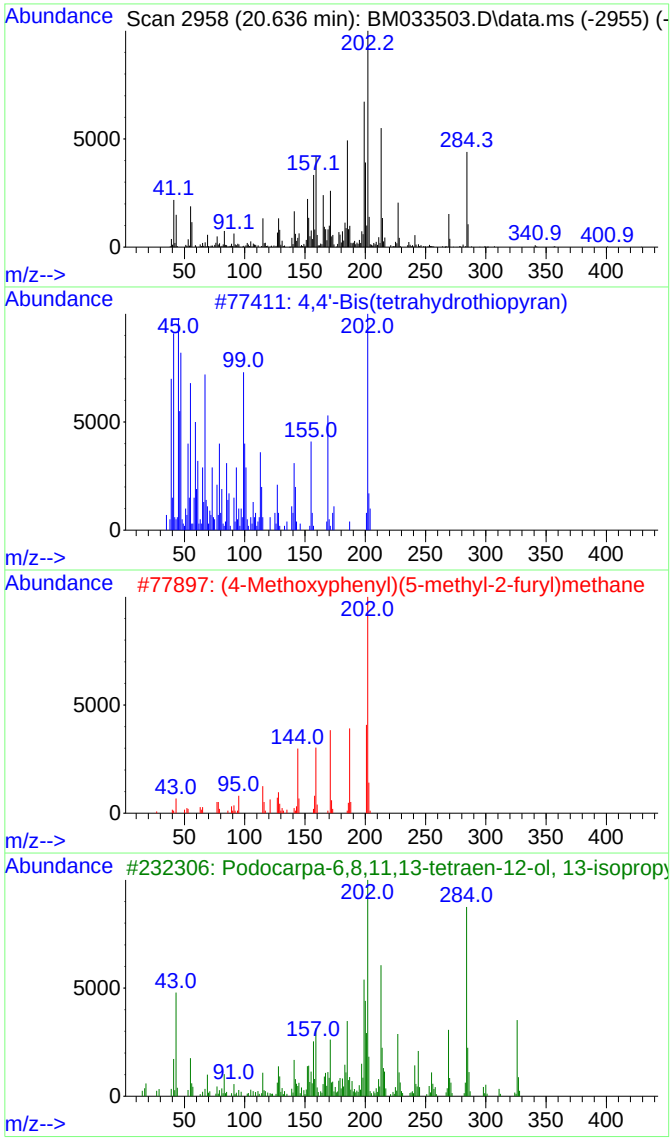
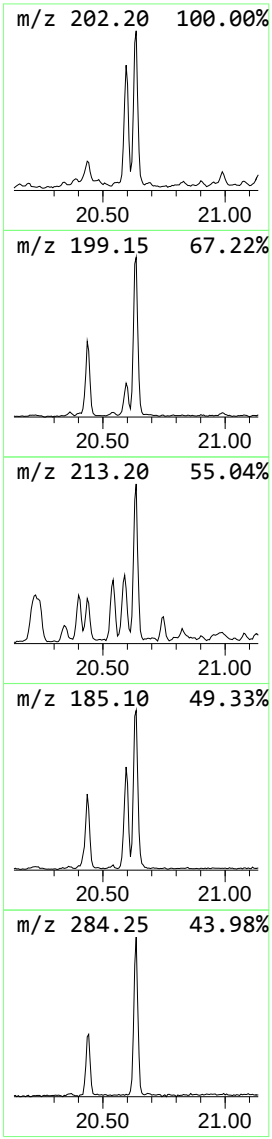
****
Peak Number 16 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.636	18.22 ng	1137940	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	90
2	(4-Methoxyphenyl)(5-methyl-2-fur...	202	C13H14O2	1000440-64-7	35
3	Podocarpa-6,8,11,13-tetraen-12-o...	326	C22H30O2	022160-86-7	27
4	Fluoren-9-one, 9a-hydroxy-1,2,3,...	202	C13H14O2	1000160-37-9	25
5	1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	20





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Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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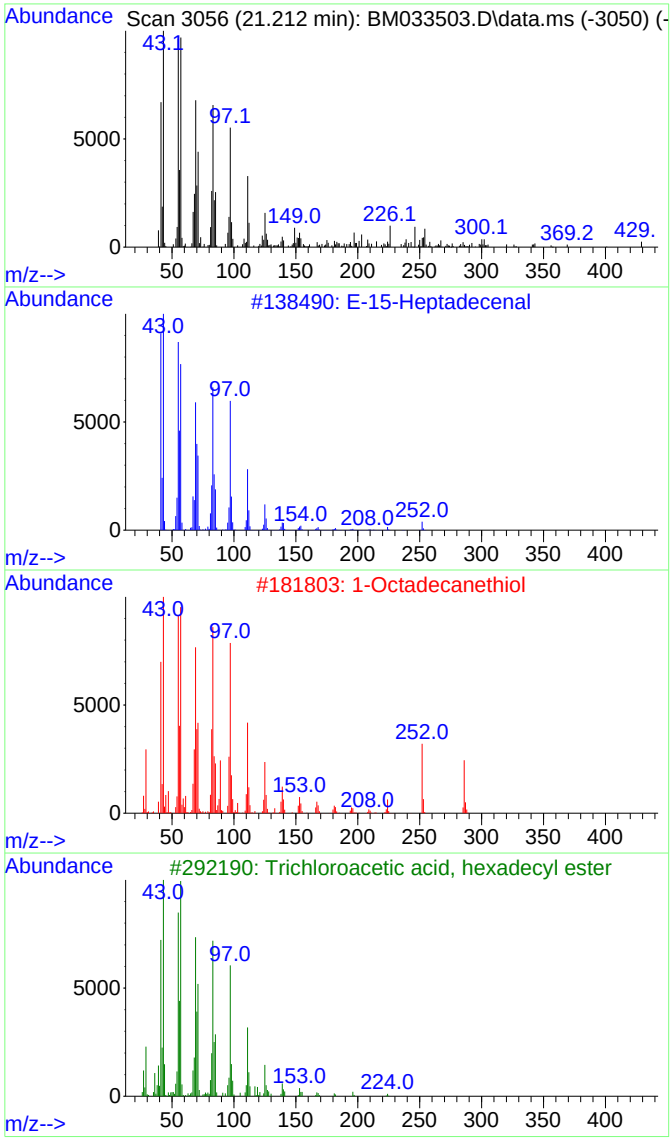
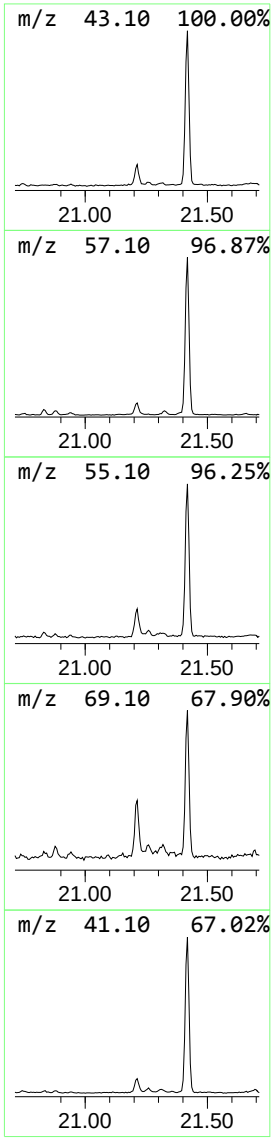
Peak Number 17 E-15-Heptadecenal Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.212	6.21 ng	388224	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	96
2	1-Octadecanethiol	286	C18H38S	002885-00-9	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	1-Docosene	308	C22H44	001599-67-3	91





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Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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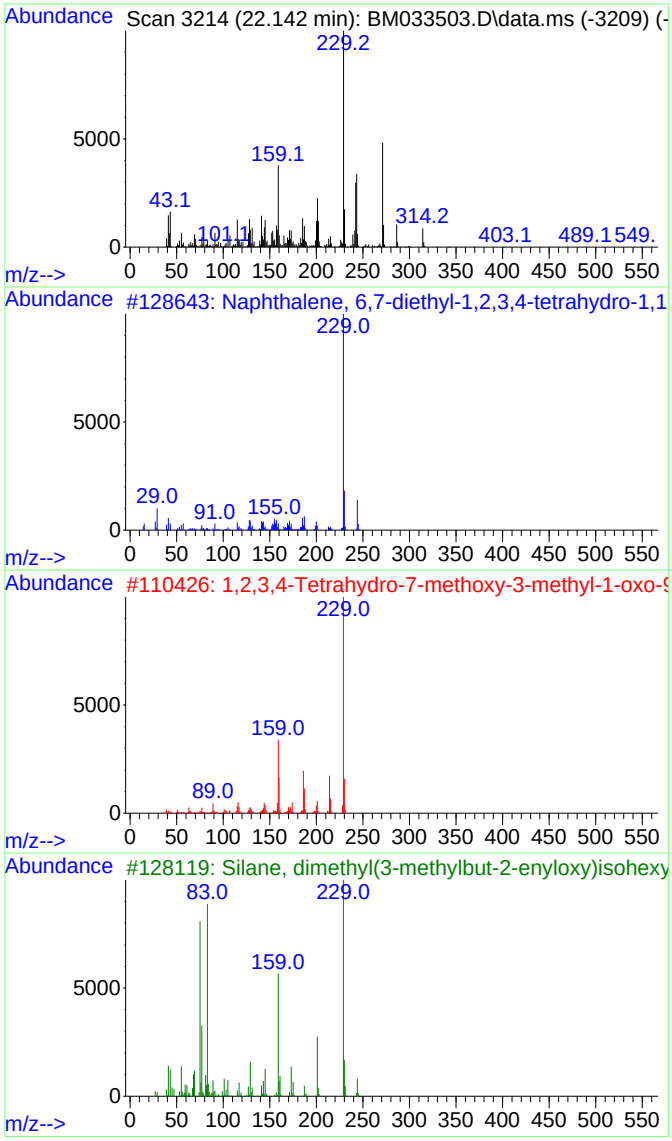
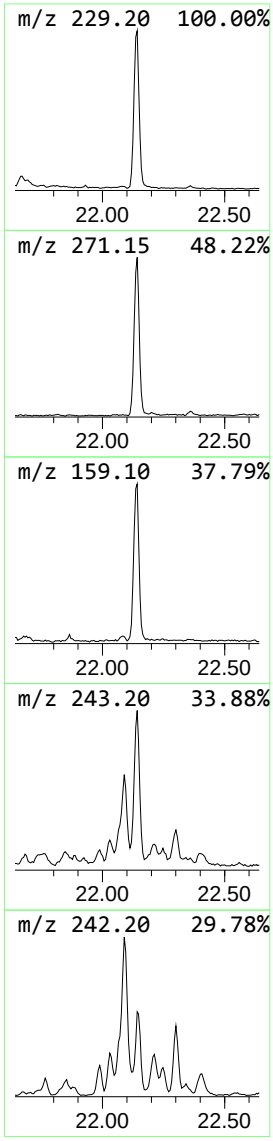
Peak Number 18 Naphthalene, 6,7-diethyl-1,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.142	18.02 ng	1125640	Chrysene-d12	21.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 6,7-diethyl-1,2,3,4...	244	C18H28	055741-10-1	52
2	1,2,3,4-Tetrahydro-7-methoxy-3-m...	229	C14H15NO2	032550-51-9	46
3	Silane, dimethyl(3-methylbut-2-e...	244	C13H28O2Si	1010347-96-5	43
4	Silane, methylvinyl(4-methylpent...	286	C16H34O2Si	1010416-96-5	38
5	N-(7-Chloro-2-phenazinyl)acetamide	271	C14H10ClN3O	023677-13-6	32





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Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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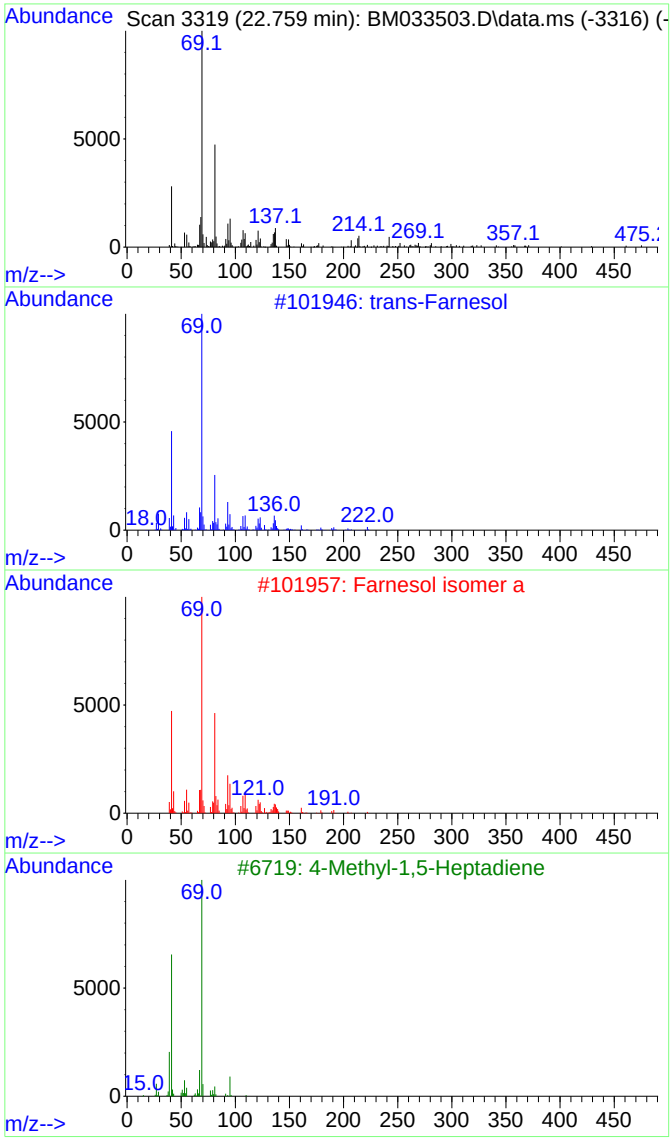
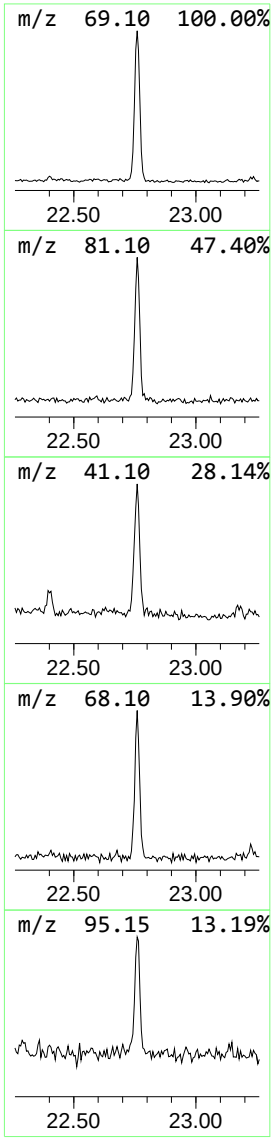
Peak Number 19 trans-Farnesol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.759	23.02 ng	362741	Perylene-d12	23.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Farnesol	222	C15H26O	000106-28-5	76
2	Farnesol isomer a	222	C15H26O	1000108-92-4	74
3	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	72
4	2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	64
5	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	64





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Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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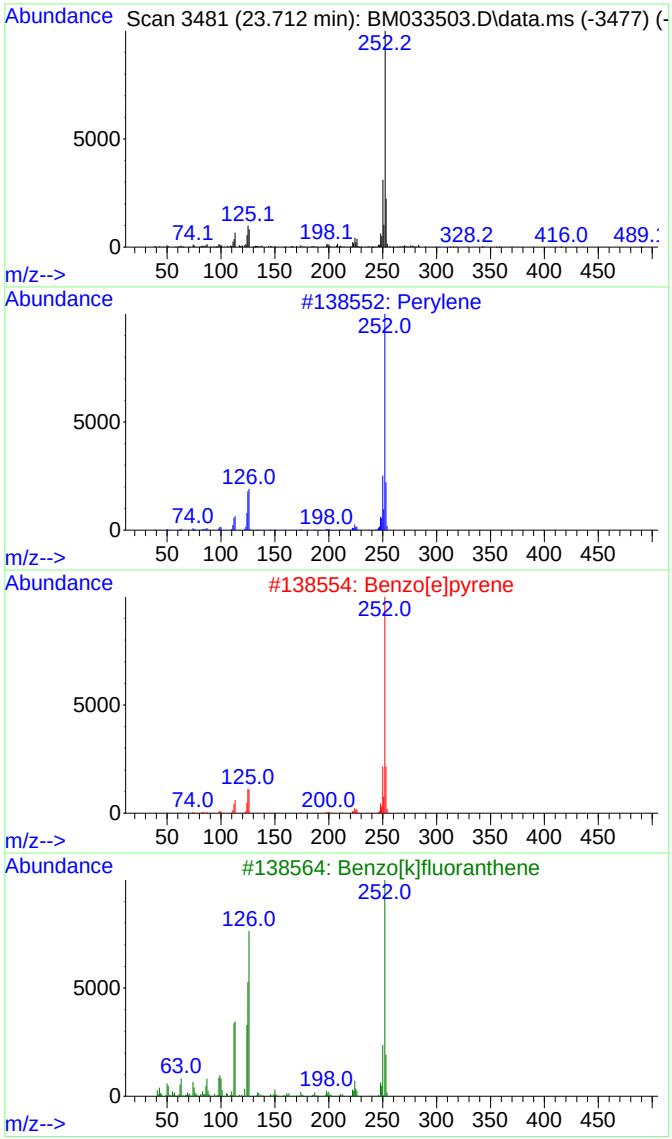
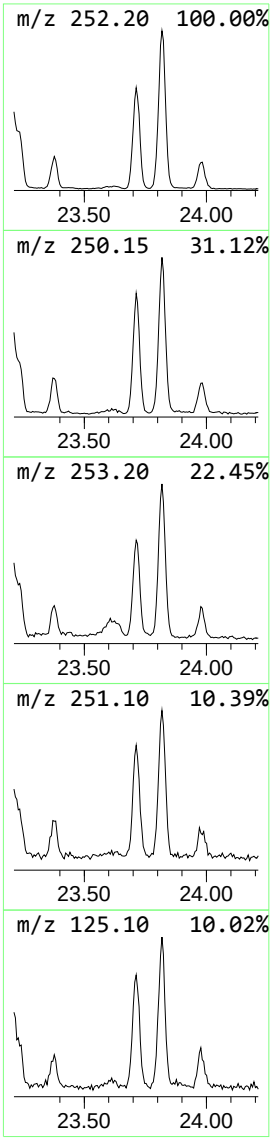
Peak Number 20 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.712	31.05 ng	489230	Perylene-d12	23.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[e]pyrene	252	C20H12	000192-97-2	94
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121721\
Data File : BM033503.D
Acq On : 17 Dec 2021 13:09
Operator : CG/JU
Sample : M5089-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MS-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM121621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.037	36.8	ng	676250	1	7.931	367869	20.0
3-Isopropyl-6,8...	13.360	7.6	ng	258220	3	14.583	676787	20.0
Longifolene	13.848	70.0	ng	2368610	3	14.583	676787	20.0
1H-3a,7-Methano...	13.895	12.7	ng	429777	3	14.583	676787	20.0
cis-Thujopsene	14.101	6.7	ng	227968	3	14.583	676787	20.0
Benzene, 1-meth...	14.830	8.4	ng	283828	3	14.583	676787	20.0
1H-Benzocyclohe...	15.813	6.0	ng	202060	3	14.583	676787	20.0
Cedrol	15.866	37.3	ng	1262770	3	14.583	676787	20.0
n-Hexadecanoic ...	18.218	6.5	ng	239294	4	17.330	734107	20.0
9,10-Dimethylan...	19.124	6.1	ng	224970	4	17.330	734107	20.0
Cyclopenta(def)...	19.265	6.2	ng	228976	4	17.330	734107	20.0
Pyrene, 1-methyl-	20.224	8.9	ng	554482	5	21.506	1249370	20.0
unknown20.436	20.436	13.1	ng	817490	5	21.506	1249370	20.0
Pyrene, 4-methyl-	20.542	5.9	ng	368309	5	21.506	1249370	20.0
2-Phenanthrenol...	20.595	66.5	ng	4153310	5	21.506	1249370	20.0
4,4'-Bis(tetrah...	20.636	18.2	ng	1137940	5	21.506	1249370	20.0
E-15-Heptadecenal	21.212	6.2	ng	388224	5	21.506	1249370	20.0
Naphthalene, 6,...	22.142	18.0	ng	1125640	5	21.506	1249370	20.0
trans-Farnesol	22.759	23.0	ng	362741	6	23.924	315175	20.0
Perylene	23.712	31.1	ng	489230	6	23.924	315175	20.0