LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

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-BM102123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042485.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.705	84	88	94	rVB	119319	148200	2.67%	0.246%
2	5.093	319	324	334	rVB	284887	381979	6.89%	0.634%
3	5.293	352	358	367	rVB3	62448	93888	1.69%	0.156%
4	5.528	387	398	413	rBV	289037	527506	9.51%	0.875%
5	5.869	449	456	464	rVV2	94291	156258	2.82%	0.259%
6	6.051	477	487	496	rVB2	113574	194915	3.52%	0.323%
7	6.275	518	525	533	rBV	77360	141260	2.55%	0.234%
8	7.163	668	676	678	rBV	204259	356667	6.43%	0.592%
9	7.187	678	680	688	rVB	219047	317028	5.72%	0.526%
10	7.416	713	719	728	rVB5	47828	124377	2.24%	0.206%
11	7.528	731	738	743	rBV	123849	188077	3.39%	0.312%
12	7.581	743	747	751	rBV	92319	133610	2.41%	0.222%
13	7.687	758	765	766	rBV2	58797	91377	1.65%	0.152%
14	7.757	771	777	786	rVV	1205720	2032160	36.65%	3.371%
15	7.922	802	805	810	rVV	114123	154061	2.78%	0.256%
16	7.981	810	815	821	rVV2	466378	803672	14.50%	1.333%
17	8.028	821	823	830	rVB	67719	83356	1.50%	0.138%
18	8.151	838	844	858	rVB	2112372	3384144	61.04%	5.614%
19	8.440	887	893	910	rBV3	64667	158172	2.85%	0.262%
20	8.722	930	941	945	rBV2	86980	189294	3.41%	0.314%
21	8.787	945	952	959	rVV2	724021	1241156	22.39%	2.059%
22	9.104	999	1006	1013	rBV	146676	254278	4.59%	0.422%
23	9.187	1013	1020	1025	rVV	725160	1225284	22.10%	2.033%
24	9.228	1025	1027	1032	rVV	166748	234897	4.24%	0.390%
25	9.292	1032	1038	1045	rVB	115999	224273	4.05%	0.372%
26	9.410	1053	1058	1075	rVB3	106298	298520	5.38%	0.495%
27	9.557	1075	1083	1085	rBV4	38325	83940	1.51%	0.139%
28	9.604	1085	1091	1093	rVV	285219	542765	9.79%	0.900%
29	9.639	1093	1097	1103	rVV	435186	746667	13.47%	1.239%
30	9.692	1103	1106	1114	rVB3	42410	81491	1.47%	0.135%
31	9.904	1137	1142	1148	rBV	41158	81617	1.47%	0.135%
32	10.081	1167	1172	1174	rBV2	134430	209802	3.78%	0.348%
33	10.128	1174	1180	1191	rVV	982791	1689012	30.46%	2.802%
34	10.228	1191	1197	1203	rVV2	383810	648243	11.69%	1.075%
35	10.334	1203	1215	1220	rVV3	347016	840960	15.17%	1.395%
36	10.392	1220	1225	1230	rVV2	169657	313528	5.65%	0.520%

LSC Area Percent Report

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Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LCOL-12

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-BM102123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.581	1252	1257	1261	rBV	149973	255499	4.61%	0.424%
38	10.633	1261	1266	1271	rVV6	71935	187194	3.38%	0.311%
39	10.710	1272	1279	1282	rVB6	67016	150135	2.71%	0.249%
40	10.804	1287	1295	1299	rVV	667907	1315807	23.73%	2.183%
41	10.851	1299	1303	1310	rVB	457272	751196	13.55%	1.246%
42	11.016	1319	1331	1336	rBV	238714	543880	9.81%	0.902%
43	11.081	1338	1342	1349	rVB3	116993	214602	3.87%	0.356%
44	11.186	1352	1360	1365	rBV3	350263	769939	13.89%	1.277%
45	11.310	1376	1381	1386	rBV	297714	446653	8.06%	0.741%
46	11.369	1386	1391	1402	rVB2	425116	771850	13.92%	1.280%
47	11.445	1402	1404	1411	rVB5	68249	125106	2.26%	0.208%
48	11.557	1411	1423	1426	rBV9	111129	338080	6.10%	0.561%
49	11.610	1426	1432	1436	rBV5	104517	267212	4.82%	0.443%
50	11.769	1455	1459	1465	rBV2	132261	224896	4.06%	0.373%
51	11.839	1465	1471	1476	rBV6	79582	162533	2.93%	0.270%
52	11.933	1482	1487	1491	rBV	186043	362209	6.53%	0.601%
53	12.069	1507	1510	1515	rVB3	89623	131268	2.37%	0.218%
54	12.245	1536	1540	1546	rVB2	112237	208199	3.76%	0.345%
55	12.304	1546	1550	1560	rVB3	109011	239326	4.32%	0.397%
56	12.492	1577	1582	1588	rBV4	74279	171079	3.09%	0.284%
57	12.563	1588	1594	1599	rVB	241049	391997	7.07%	0.650%
58	12.739	1618	1624	1632	rVB8	49638	119395	2.15%	0.198%
59	12.816	1632	1637	1647	rVB3	180460	332942	6.01%	0.552%
60	13.010	1651	1670	1675	rBV2	948269	2340473	42.21%	3.883%
61	13.057	1675	1678	1684	rVB3	106231	189232	3.41%	0.314%
62	13.251	1705	1711	1717	rVV	1632009	2376949	42.87%	3.943%
63	13.333	1717	1725	1729	rVV	699497	1191872	21.50%	1.977%
64	13.386	1729	1734	1742	rVV	298365	530294	9.56%	0.880%
65	13.486	1742	1751	1759	rVV3	421418	897433	16.19%	1.489%
66	13.698	1783	1787	1796	rBV5	54948	92247	1.66%	0.153%
67	14.269	1881	1884	1897	rVB5	100248	227286	4.10%	0.377%
68	14.439	1909	1913	1917	rVV	104258	152274	2.75%	0.253%
69	14.516	1921	1926	1931	rVV	113280	169686	3.06%	0.281%
70	14.627	1939	1945	1955	rVB	963134	1444291	26.05%	2.396%
71	14.863	1981	1985	1995	rVB	125913	211379	3.81%	0.351%
72	15.080	2017	2022	2027	rVB	391917	535489	9.66%	0.888%
73	15.157	2027	2035	2044	rBV	1436327	2408805	43.45%	3.996%
74	15.374	2062	2072	2077	rBV2	202469	373849	6.74%	0.620%
75	15.433	2077	2082	2088	rVV2	179796	295385	5.33%	0.490%
76	15.521	2093	2097	2105	rVB	97995	168448	3.04%	0.279%

LSC Area Percent Report

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Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

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

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.651	2116	2119	2124	rVB2	117006	147789	2.67%	0.245%
78	15.816	2143	2147	2155	rVB2	87655	166844	3.01%	0.277%
79	16.121	2190	2199	2204	rBV	858089	1238507	22.34%	2.055%
80	16.274	2220	2225	2236	rVV	128652	269099	4.85%	0.446%
81	16.504	2261	2264	2273	rVB	137624	191872	3.46%	0.318%
82	16.857	2320	2324	2329	rBV2	68878	108470	1.96%	0.180%
83	16.921	2330	2335	2346	rVB3	92974	171452	3.09%	0.284%
84	17.010	2346	2350	2354	rBV4	58546	84937	1.53%	0.141%
85	17.127	2365	2370	2374	rBV	326391	407063	7.34%	0.675%
86	17.233	2385	2388	2395	rVB4	100299	158645	2.86%	0.263%
87	17.380	2407	2413	2423	rBV	1027593	1496067	26.98%	2.482%
88	17.562	2440	2444	2448	rBV	185932	243810	4.40%	0.404%
89	17.627	2452	2455	2460	rVB3	63320	84999	1.53%	0.141%
90	18.233	2553	2558	2569	rBV	1211833	1644358	29.66%	2.728%
91	18.380	2579	2583	2590	rVB	352486	466629	8.42%	0.774%
92	18.462	2593	2597	2604	rBV2	110645	206210	3.72%	0.342%
93	18.545	2604	2611	2618	rBV	3795934	5544364	100.00%	9.198%
94	18.609	2618	2622	2630	rVB	830855	1090837	19.67%	1.810%
95	19.504	2770	2774	2781	rBV	479293	635579	11.46%	1.054%
96	19.645	2795	2798	2804	rVB3	82879	109042	1.97%	0.181%
97	19.821	2825	2828	2834	rVB	147395	181520	3.27%	0.301%
98	19.986	2851	2856	2862	rBV	1968136	2380574	42.94%	3.949%
99	21.215	3061	3065	3074	rBV2	976557	1584385	28.58%	2.628%
100	21.556	3119	3123	3133	rBV	862337	1204650	21.73%	1.998%

Sum of corrected areas: 60280525

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
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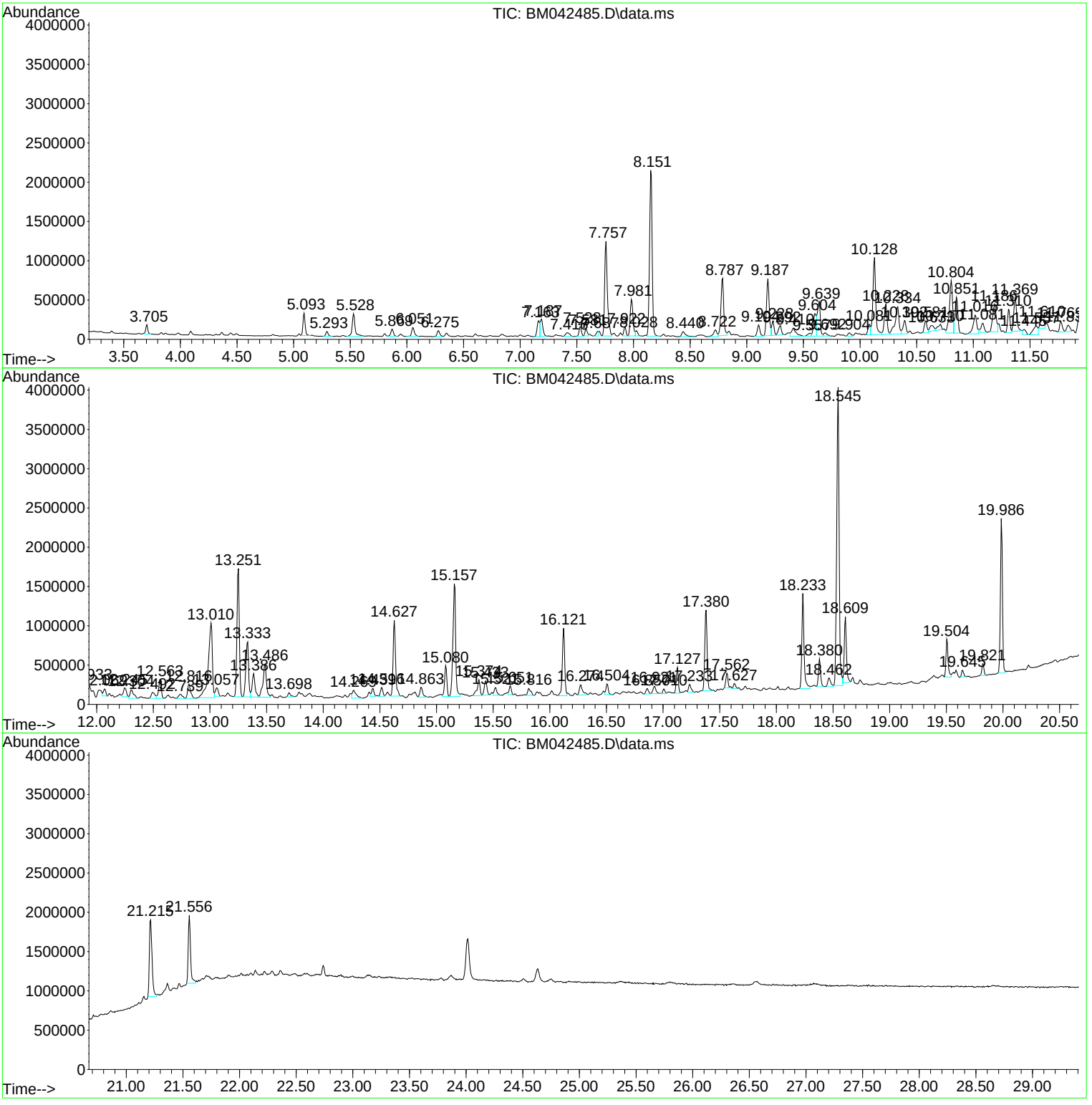
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
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BNA_M
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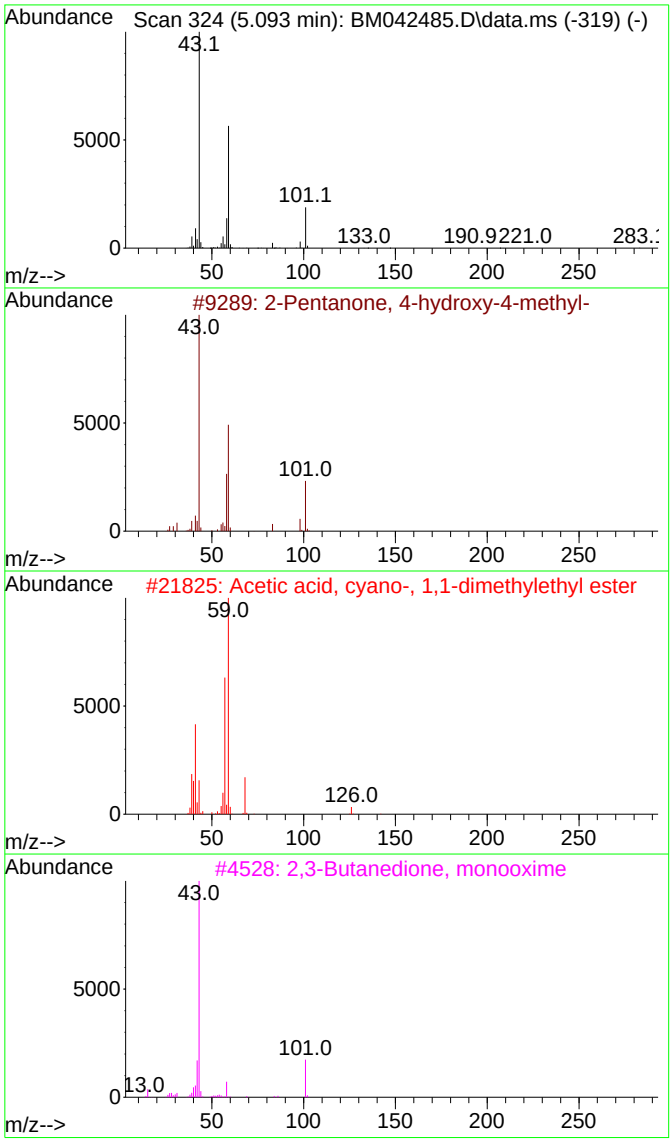
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

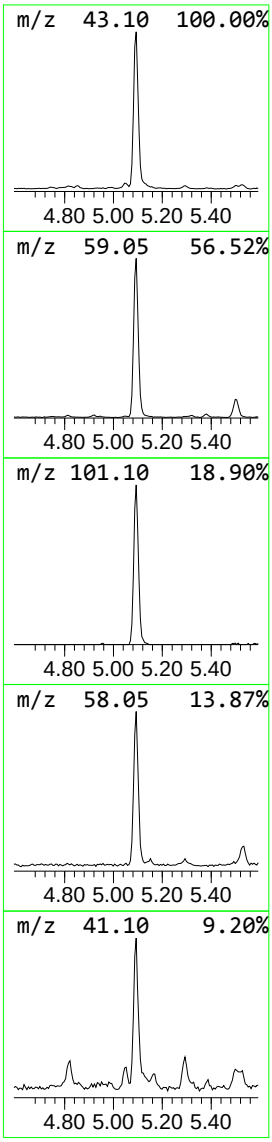
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	9.51 ng	381979	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

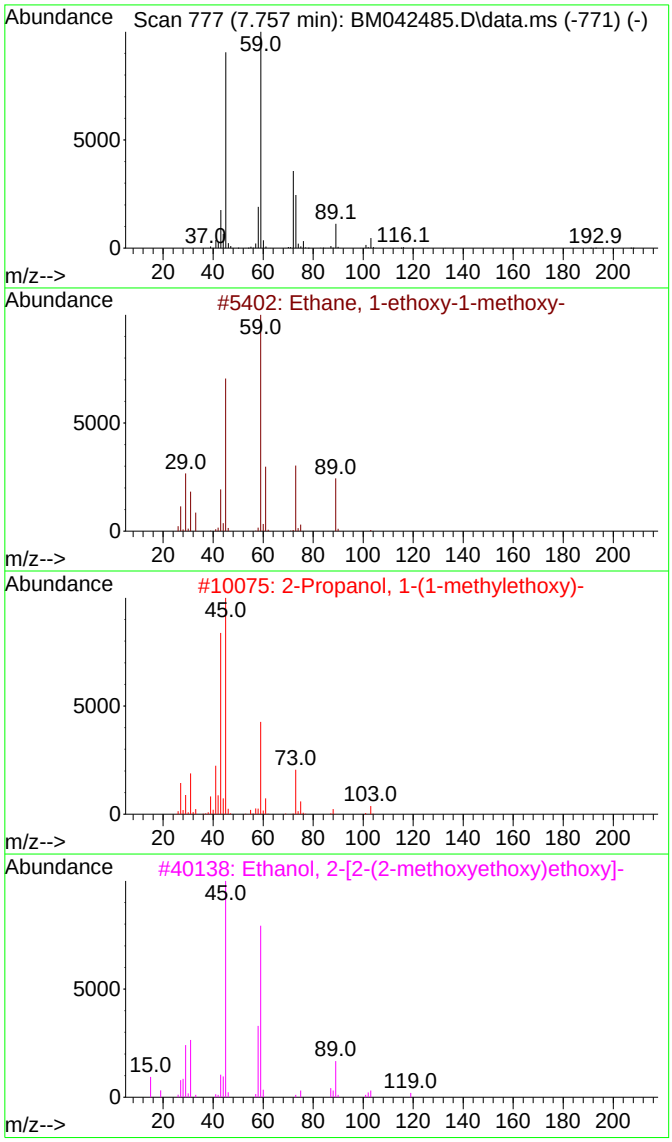
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

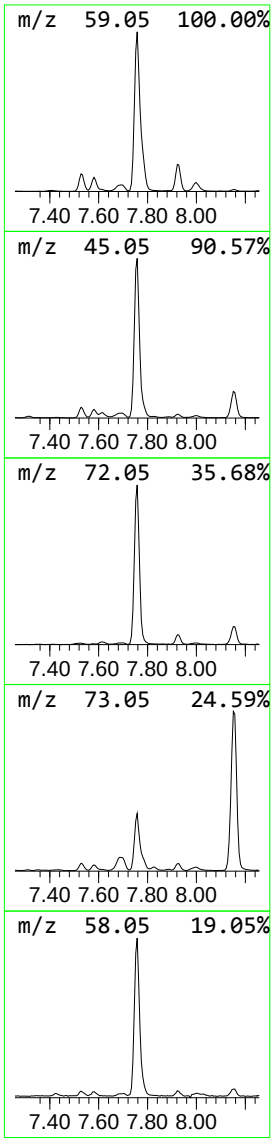
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethane, 1-ethoxy-1-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.757	50.57 ng	2032160	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	53
3	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	53
4	Diethyl carbitol	162	C8H18O3	000112-36-7	47
5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

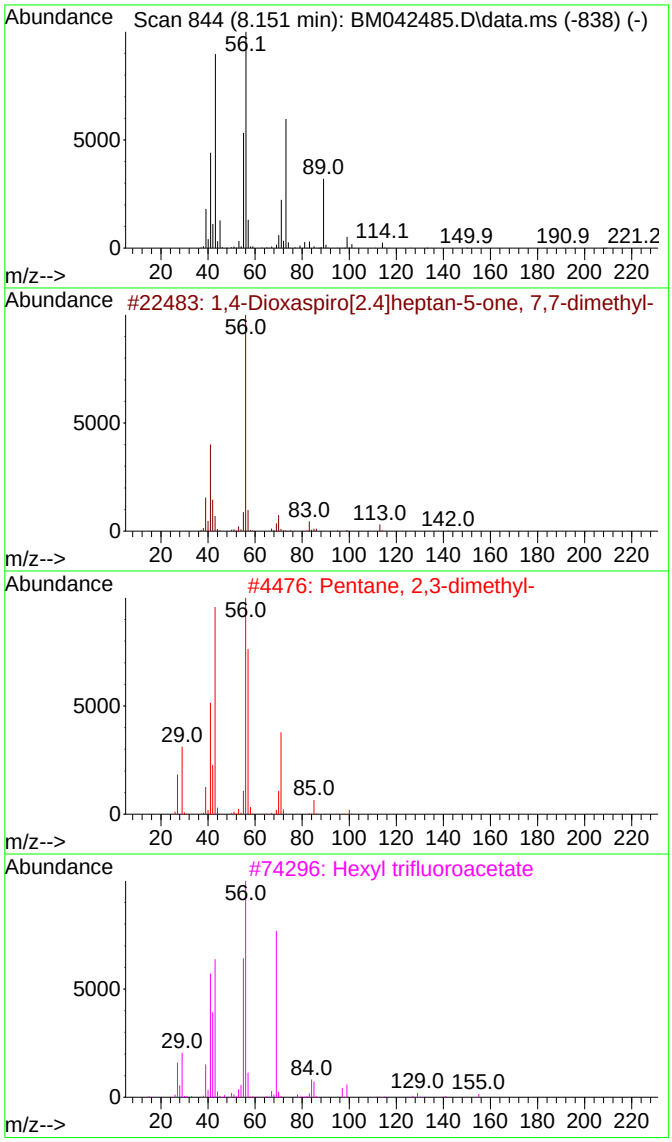
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

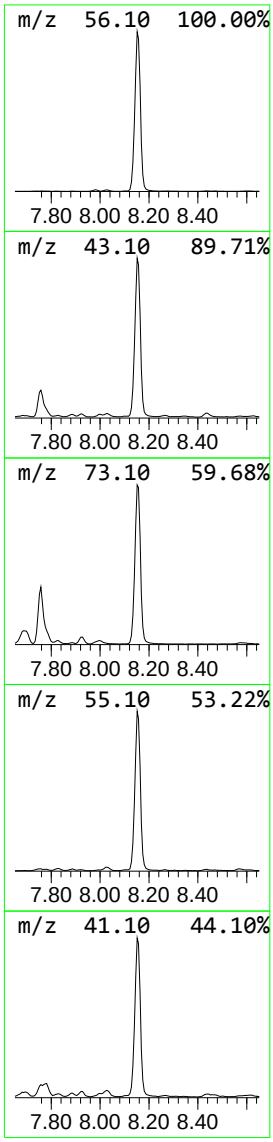
****

Peak Number 3 unknown8.151 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.151	84.22 ng	3384140	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxaspiro[2.4]heptan-5-one,...	142	C7H10O3	126091-79-0	43
2	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	38
3	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	28
4	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	28
5	2(3H)-Furanone, dihydro-3,3-dime...	114	C6H10O2	003709-08-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

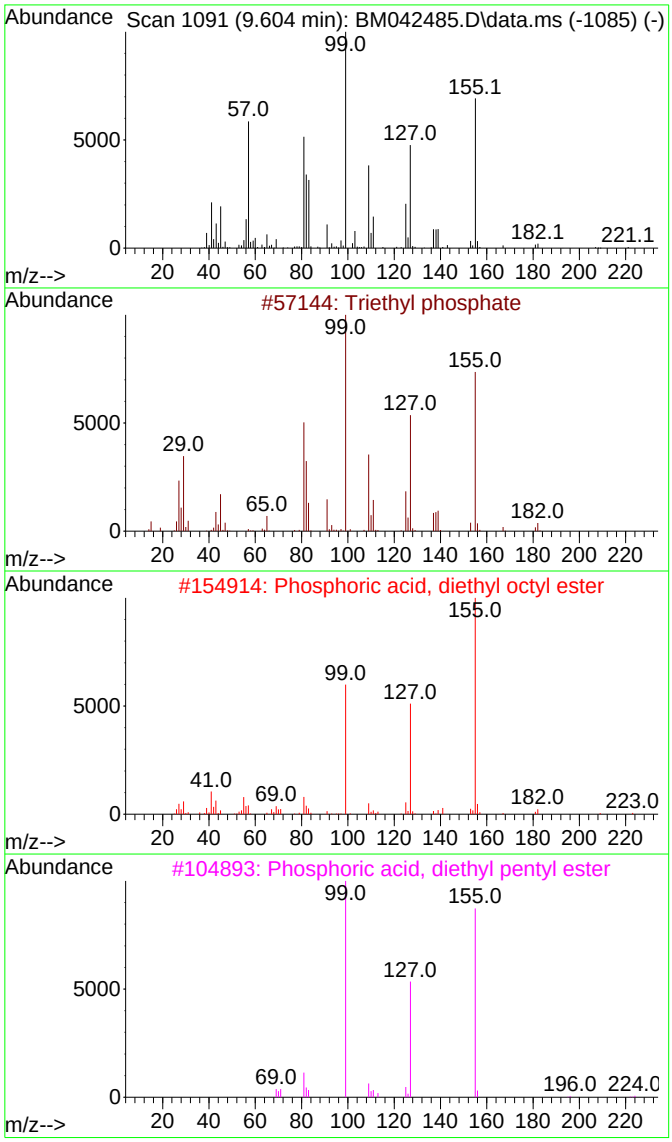
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

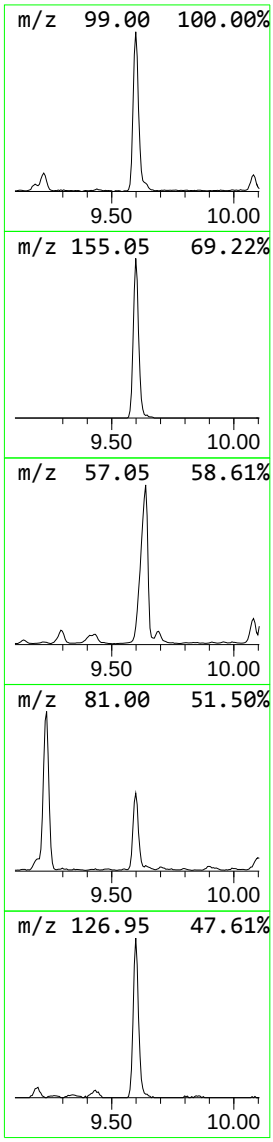
****

Peak Number 4 Triethyl phosphate Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	8.25 ng	542765	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl phosphate	182	C6H15O4P	000078-40-0	95
2	Phosphoric acid, diethyl octyl e...	266	C12H27O4P	1000308-90-4	47
3	Phosphoric acid, diethyl pentyl ...	224	C9H21O4P	020195-08-8	40
4	Butyl diethyl phosphate	210	C8H19O4P	1000298-58-0	40
5	Phosphoric acid, diethyl dodecyl...	322	C16H35O4P	1010308-89-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

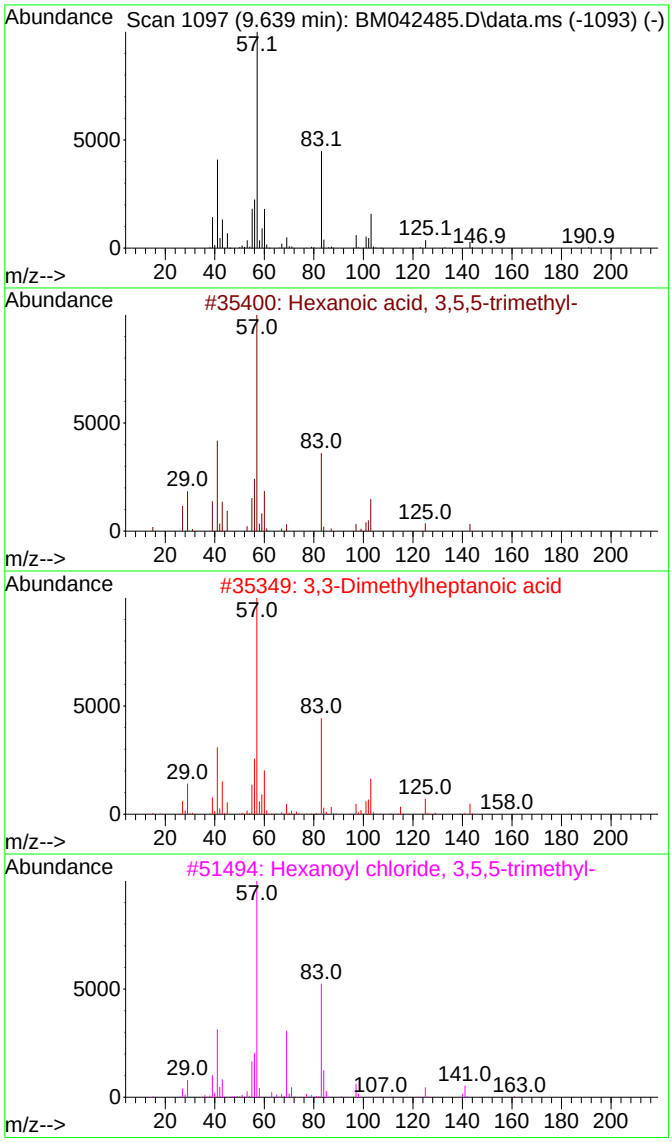
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

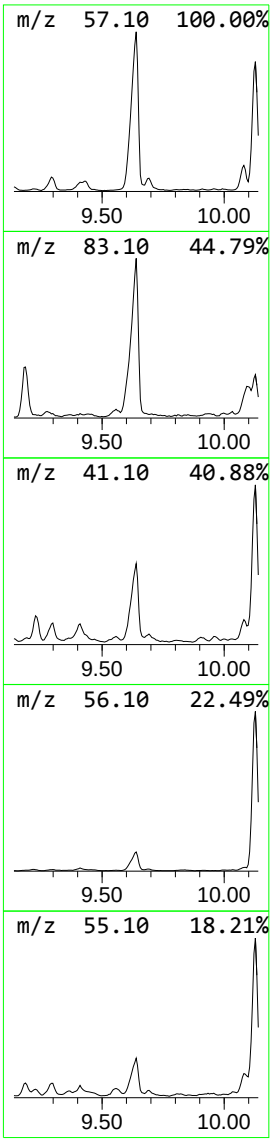
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexanoic acid, 3,5,5-trimet... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.639	11.35 ng	746667	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	83
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	42
4	6,6-Dimethylheptanoic acid	158	C9H18O2	015898-92-7	37
5	Hexanoic acid, 3,5,5-trimethyl-,...	200	C12H24O2	1000406-05-1	36





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Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

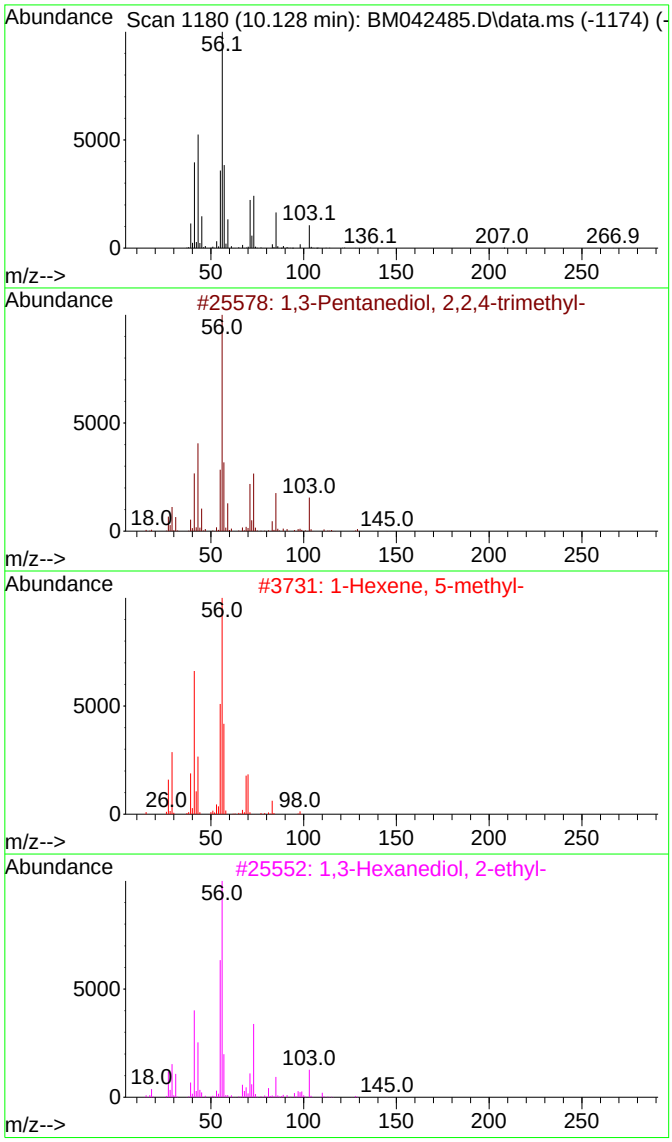
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

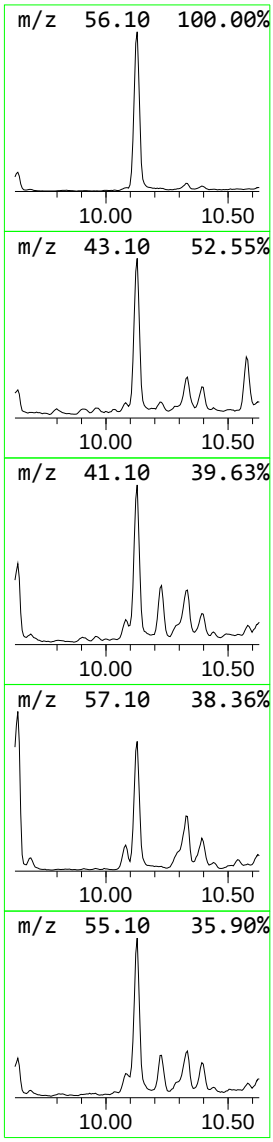
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.128	25.67 ng	1689010	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	90
2	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	32
3	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	23
4	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	23
5	1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	17





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Sample : 04909-01
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ALS Vial : 9 Sample Multiplier: 1

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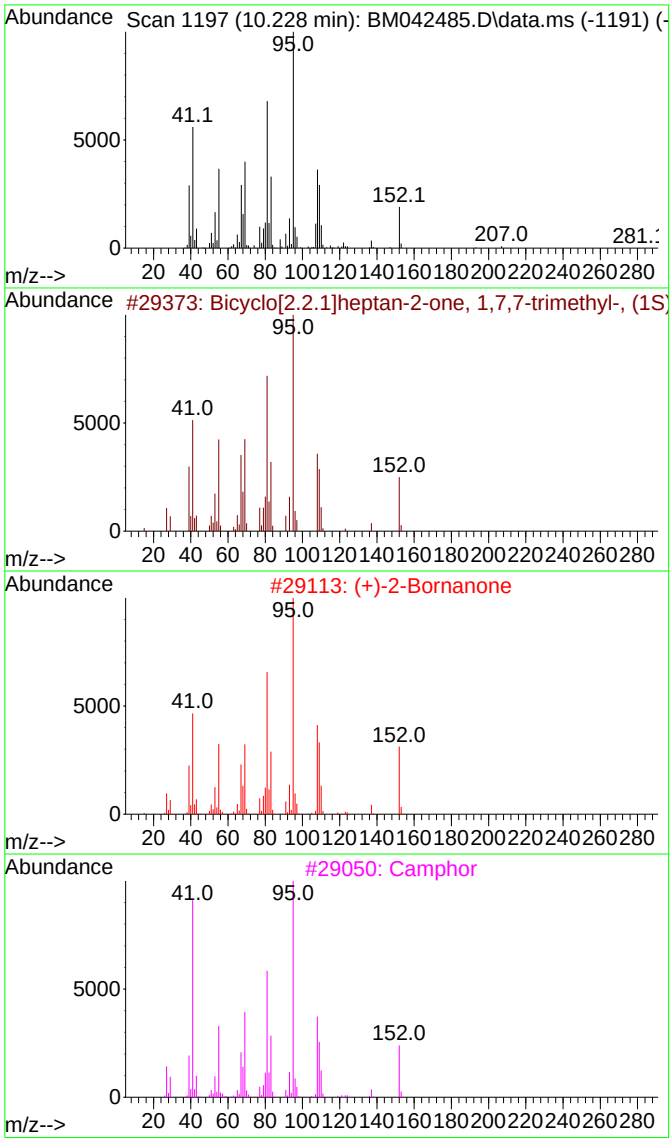
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

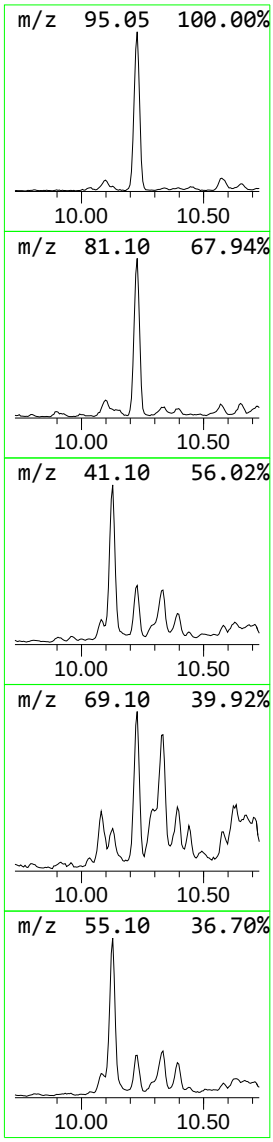
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.228	9.85 ng	648243	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3	Camphor	152	C10H16O	000076-22-2	97
4	Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152	C10H16O	062560-53-6	50
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	43





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ALS Vial : 9 Sample Multiplier: 1

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

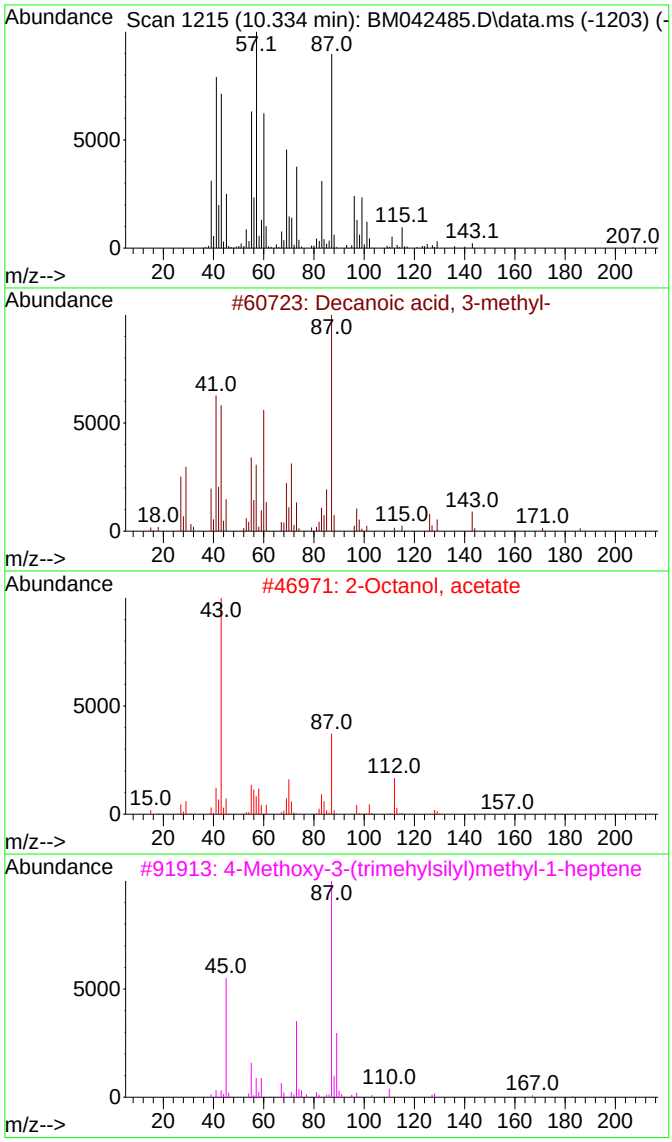
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

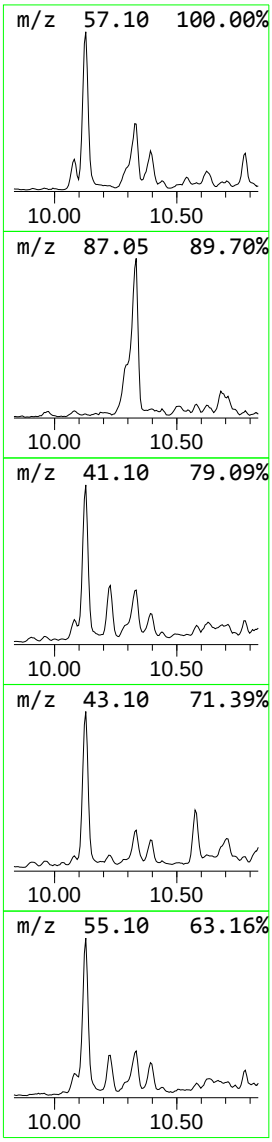
****

Peak Number 8 unknown10.334 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.334	12.78 ng	840960	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, 3-methyl-	186	C11H22O2	060308-82-9	38
2	2-Octanol, acetate	172	C10H20O2	002051-50-5	37
3	4-Methoxy-3-(trimehylsilyl)methy...	214	C12H26OSi	1000433-72-9	35
4	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	35
5	Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	35





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Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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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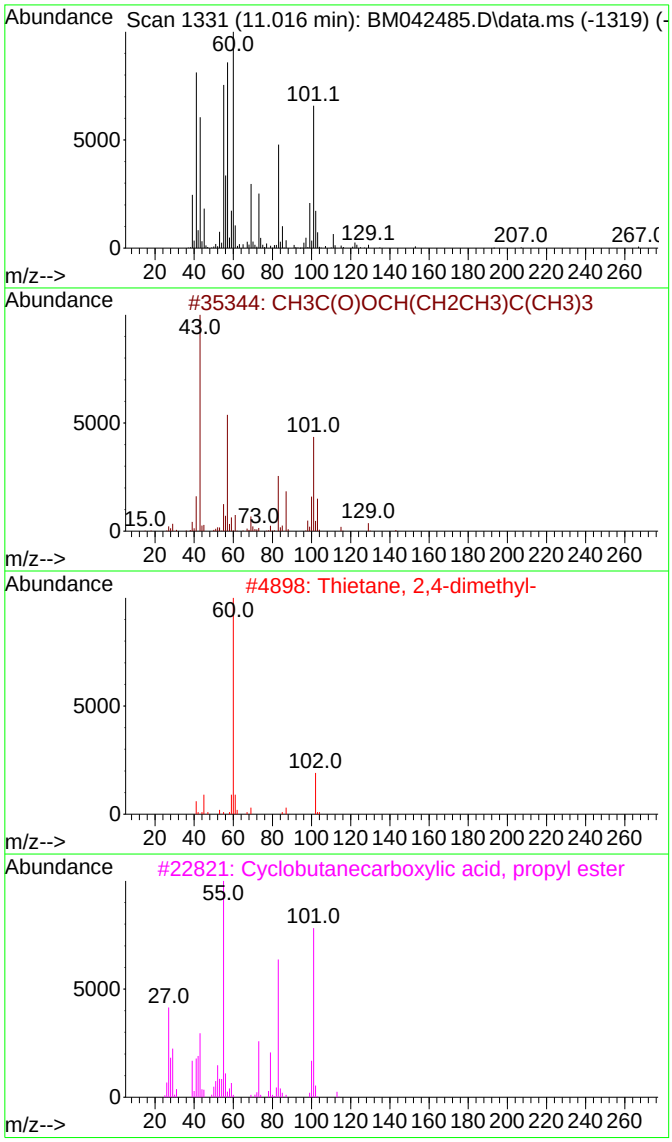
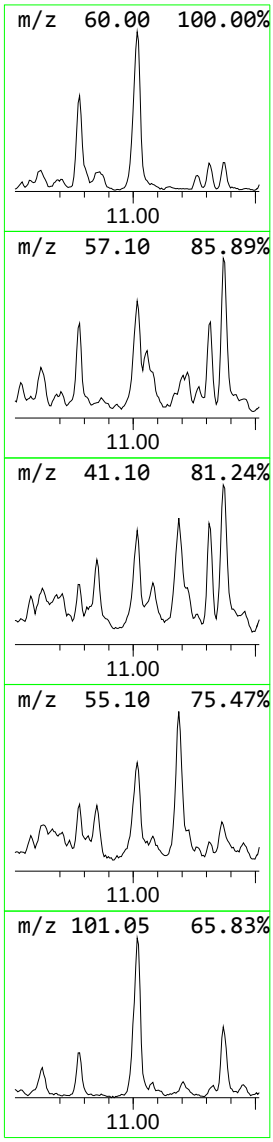
Peak Number 9 unknown11.016 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.016	8.27 ng	543880	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	CH3C(O)OCH(CH2CH3)C(CH3)3	158	C9H18O2	039511-81-4	32
2	Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	27
3	Cyclobutanecarboxylic acid, prop...	142	C8H14O2	1000280-40-0	27
4	2-Methyl-1,3-oxathiolane-2-aceti...	190	C8H14O3S	033868-62-1	27
5	Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	019467-01-7	25





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

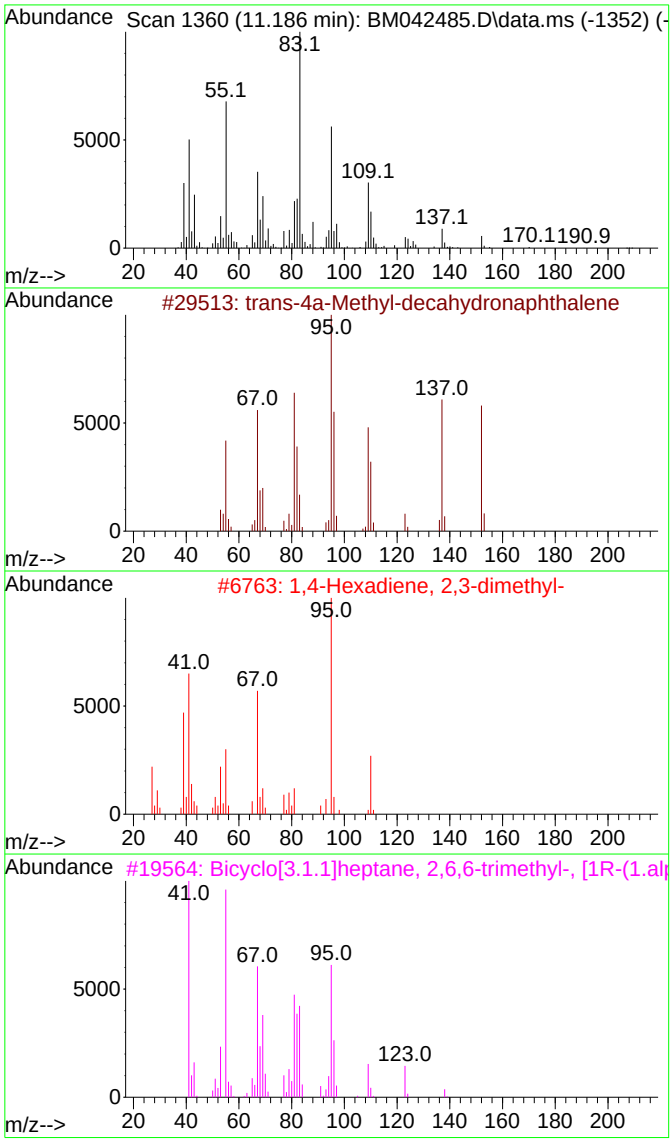
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

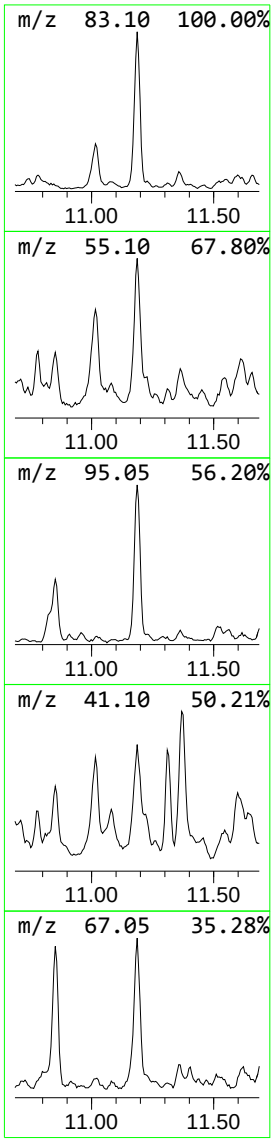
****

Peak Number 10 unknown11.186 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.186	11.70 ng	769939	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	49
2	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	35
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	30
4	trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	30
5	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	27





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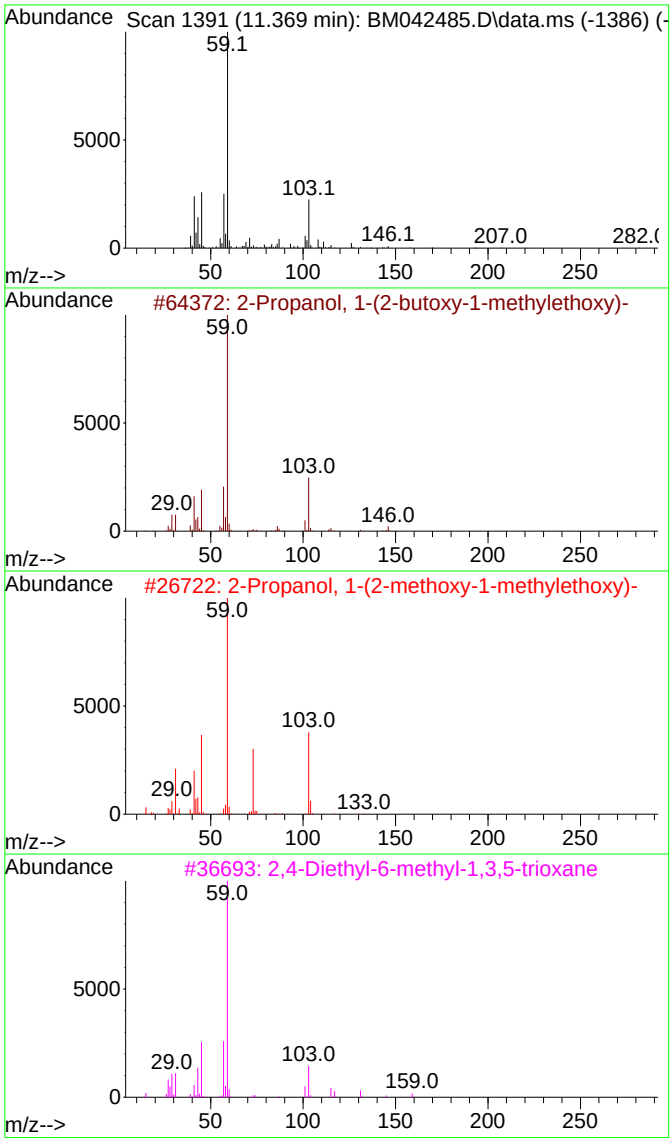
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

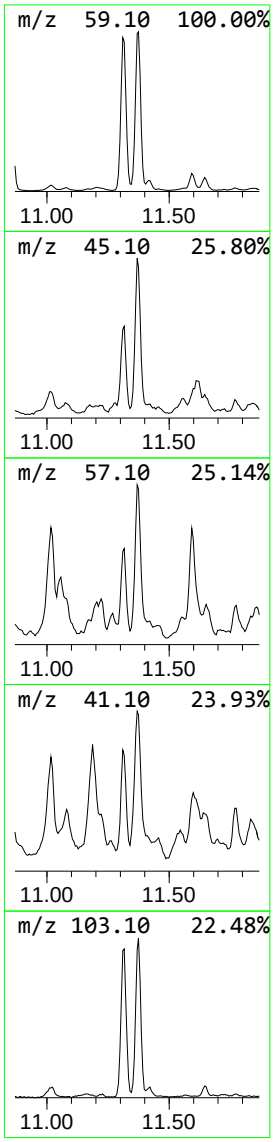
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.369	11.73 ng	771850	Naphthalene-d8	10.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	72
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
3	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	72
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
5	Methyl 2,5,8,11,14,17-hexaoxanon...	324	C14H28O8	1000366-81-4	64





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Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

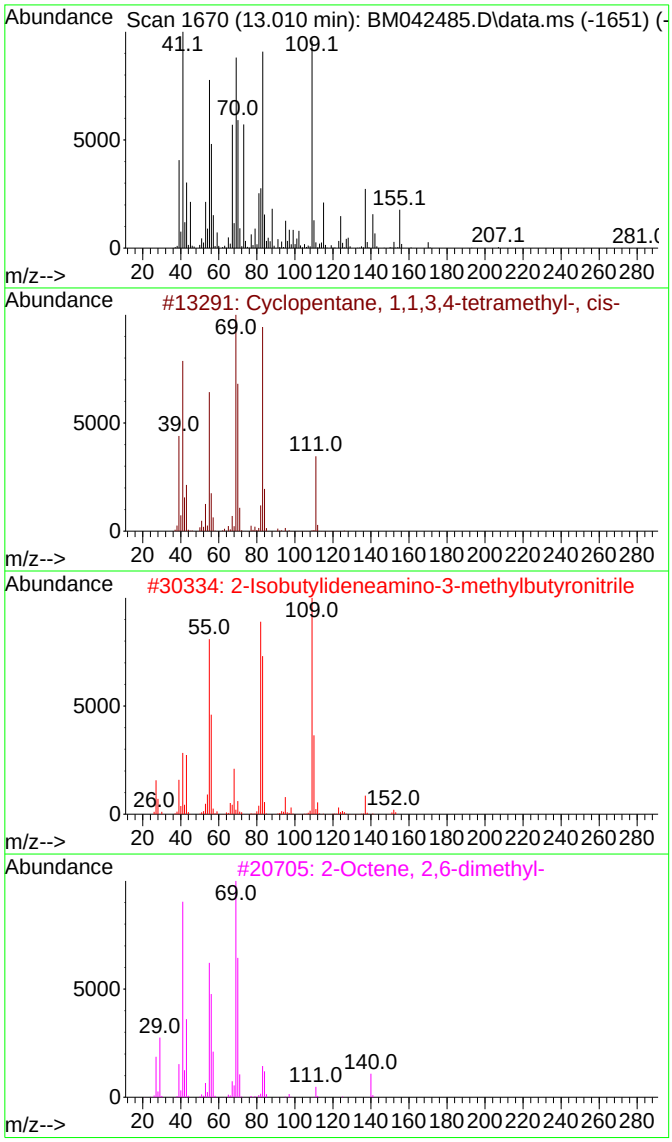
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

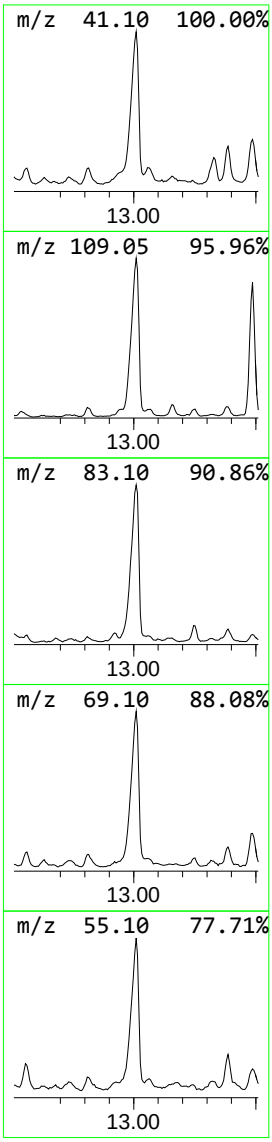
****

Peak Number 12 unknown13.010 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.010	32.41 ng	2340470	Acenaphthene-d10	14.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	053907-60-1	45
2	2-Isobutylideneamino-3-methylbut...	152	C9H16N2	125213-17-4	43
3	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	27
4	Phosphonic acid, bis(1-methyleth...	166	C6H15O3P	001809-20-7	27
5	.beta.-Citronellol, trifluoroace...	252	C12H19F3O2	1000352-29-8	22





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Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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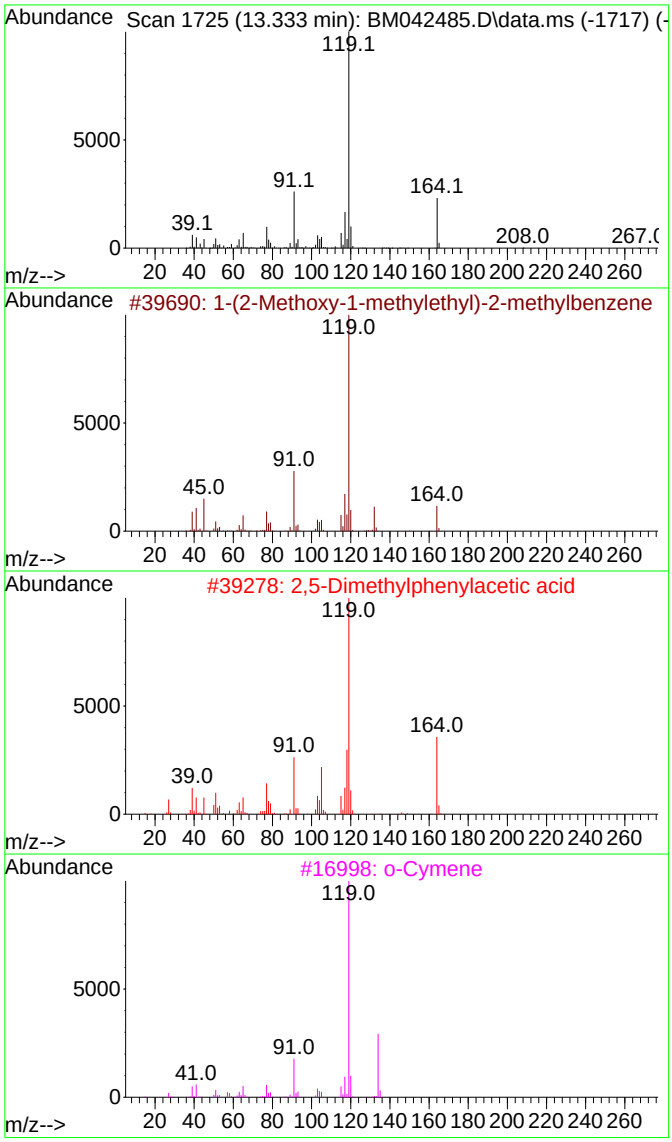
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

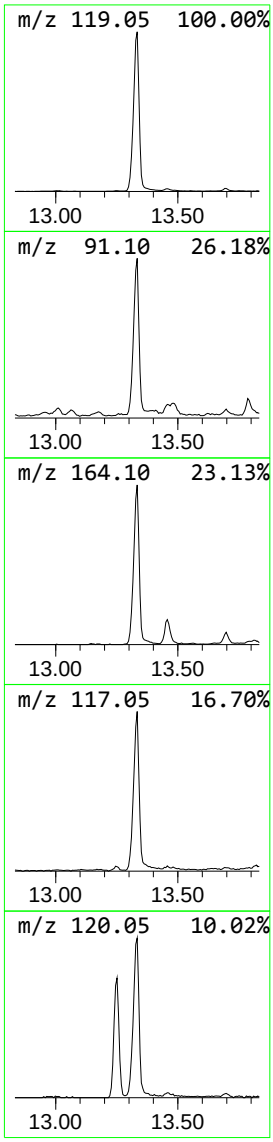
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 1-(2-Methoxy-1-methylethyl)... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	16.50 ng	1191870	Acenaphthene-d10	14.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Methoxy-1-methylethyl)-2-me...	164	C11H16O	1000210-02-1	90
2	2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	83
3	o-Cymene	134	C10H14	000527-84-4	72
4	p-Cymene	134	C10H14	000099-87-6	72
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	64





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

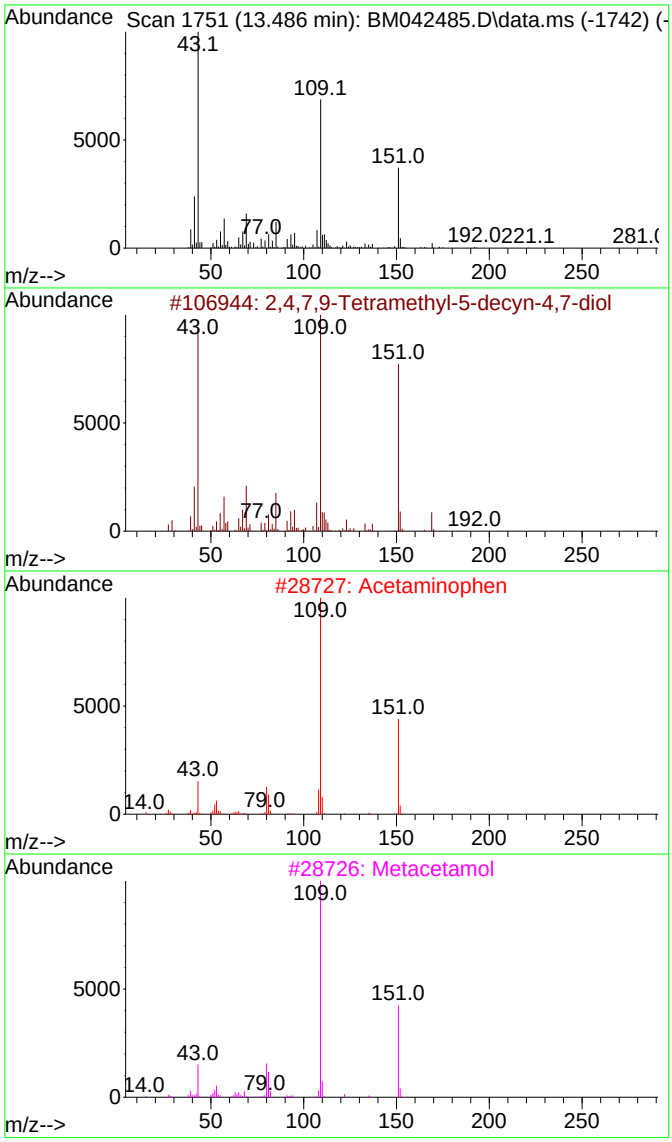
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

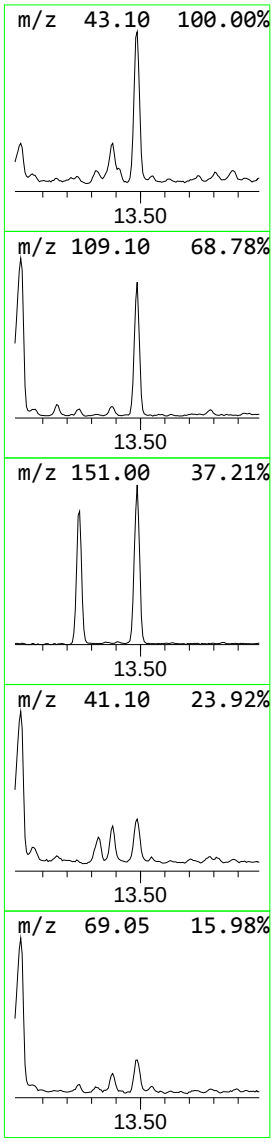
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.486	12.43 ng	897433	Acenaphthene-d10	14.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Acetaminophen	151	C8H9NO2	000103-90-2	52
3	Metacetamol	151	C8H9NO2	000621-42-1	50
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	50





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ALS Vial : 9 Sample Multiplier: 1

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BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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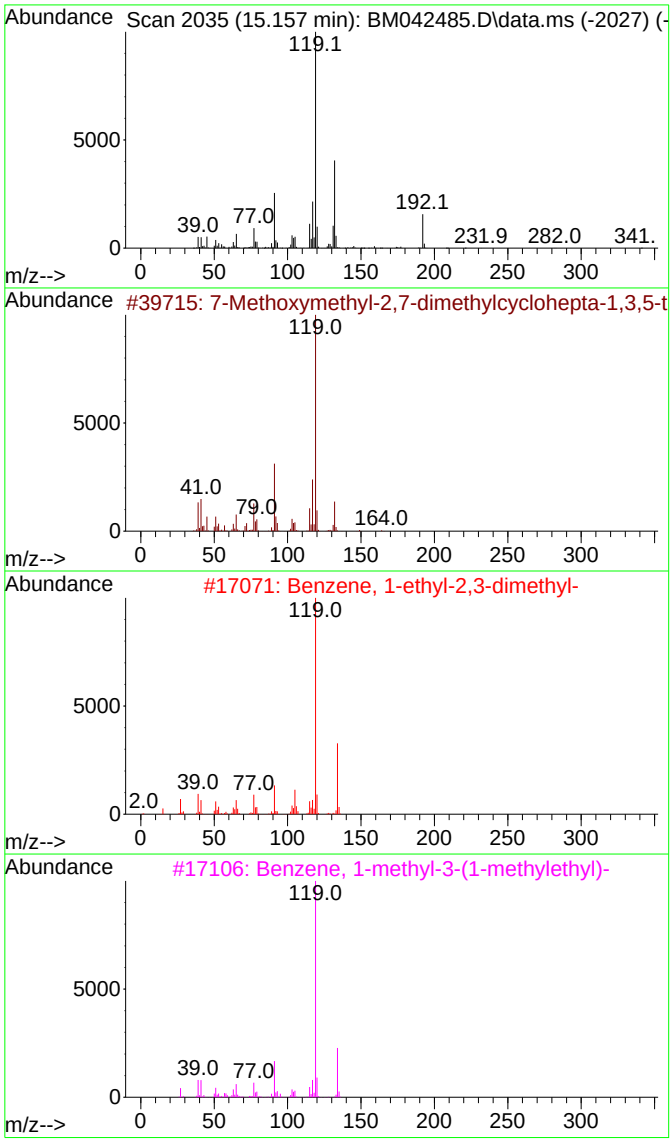
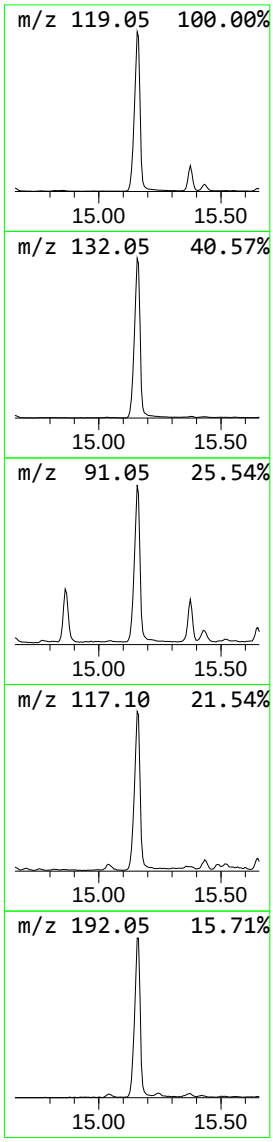
****
Peak Number 15 7-Methoxymethyl-2,7-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	33.36 ng	2408810	Acenaphthene-d10	14.627

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methoxymethyl-2,7-dimethylcycl...	164	C11H16O	073992-48-0	64
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	46
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	43
4	p-Cymene	134	C10H14	000099-87-6	43
5	Benzenebutanoic acid, 2,5-dimethyl-	192	C12H16O2	001453-06-1	43





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TIC Library : C:\Database\NIST20.L
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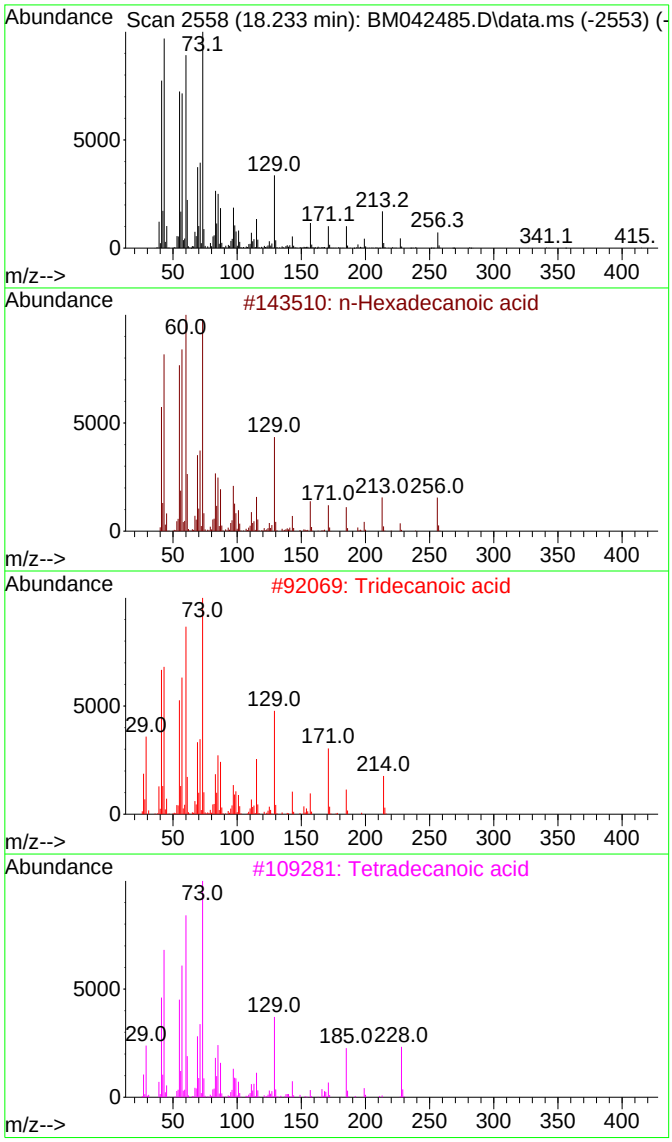
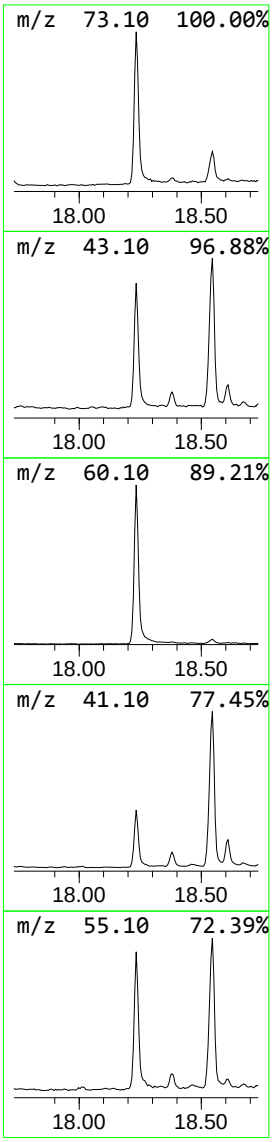
Peak Number 16 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	21.98 ng	1644360	Phenanthrene-d10	17.380

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	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

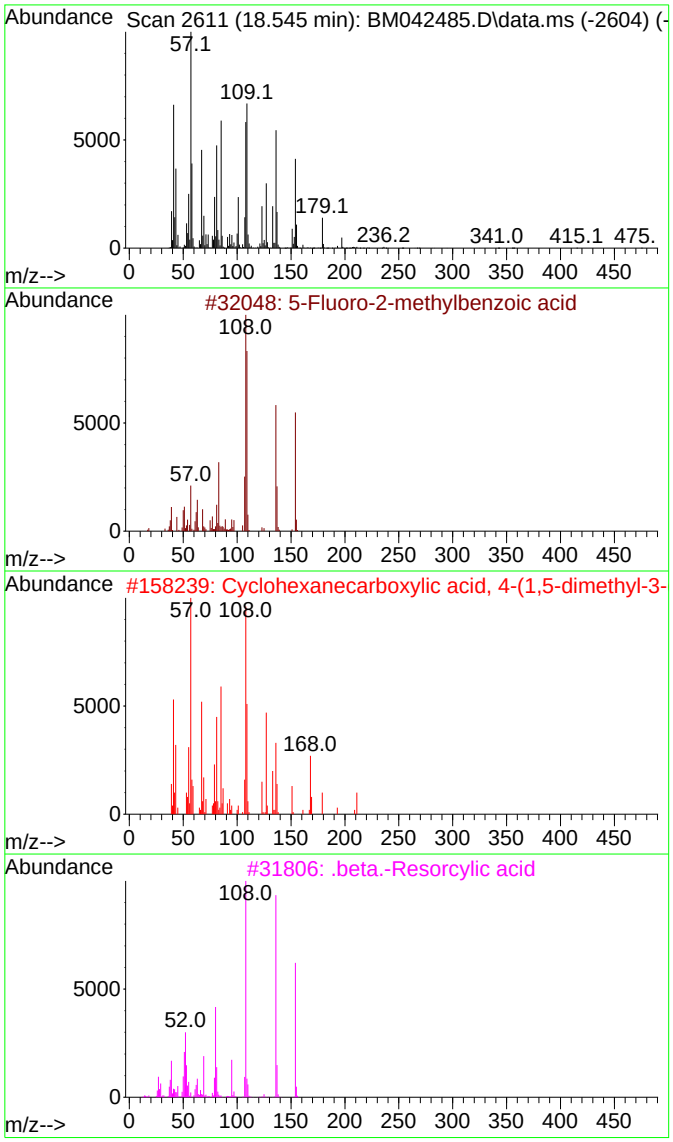
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

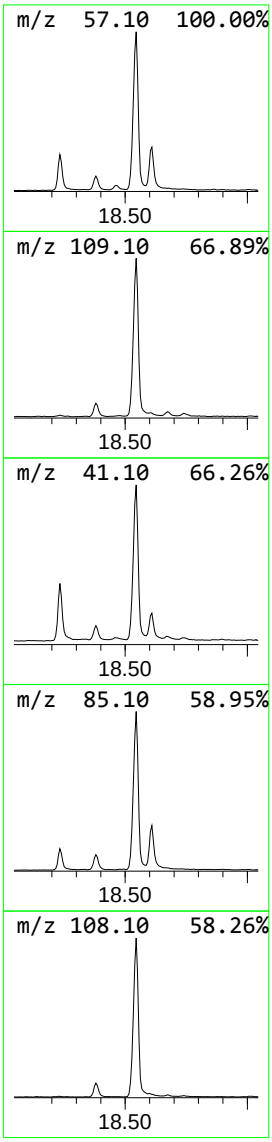
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 5-Fluoro-2-methylbenzoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.545	74.12 ng	5544360	Phenanthrene-d10	17.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methylbenzoic acid	154	C8H7FO2	033184-16-6	50
2	Cyclohexanecarboxylic acid, 4-(1...	268	C16H28O3	017904-29-9	37
3	.beta.-Resorcylic acid	154	C7H6O4	000089-86-1	30
4	1-Acetyl-1-methyl-4-methylenecyc...	152	C10H16O	1000424-28-4	16
5	1H-Pyrrole, 4-ethyl-2,3-dimethyl-	123	C8H13N	000491-18-9	14





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Data File : BM042485.D
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Operator : MA/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

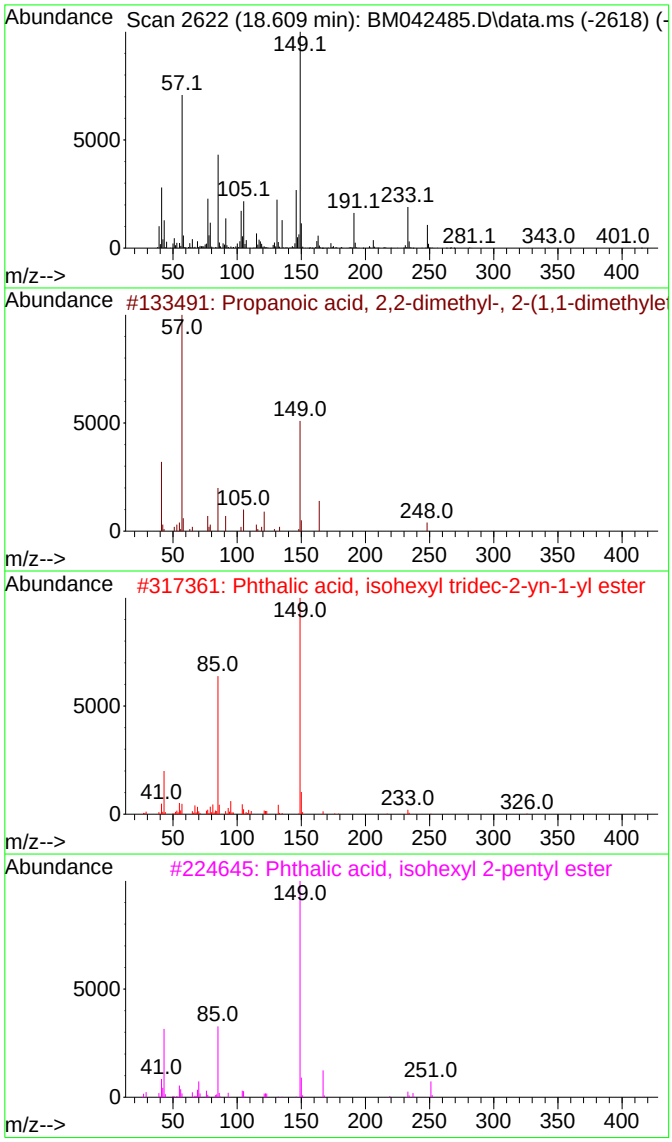
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

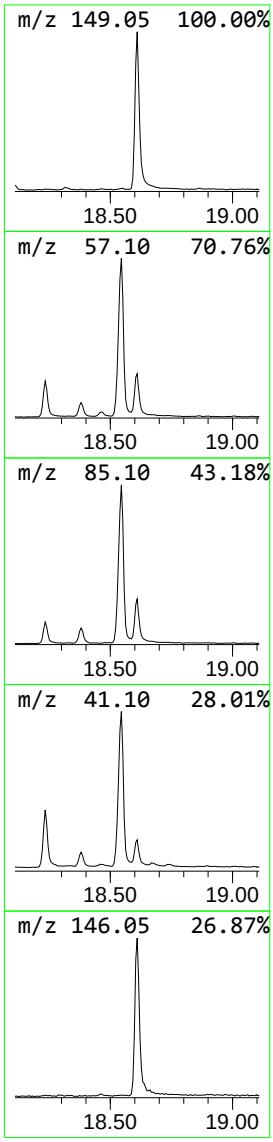
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 Propanoic acid, 2,2-dimethy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.609	14.58 ng	1090840	Phenanthrene-d10	17.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2-dimethyl-, 2...	248	C16H24O2	054644-45-0	58
2	Phthalic acid, isohexyl tridec-2...	428	C27H40O4	1000315-44-4	50
3	Phthalic acid, isohexyl 2-pentyl...	320	C19H28O4	1000315-48-7	47
4	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	38
5	Phthalic acid, 3-fluorophenyl pr...	302	C17H15FO4	1000356-49-8	35





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Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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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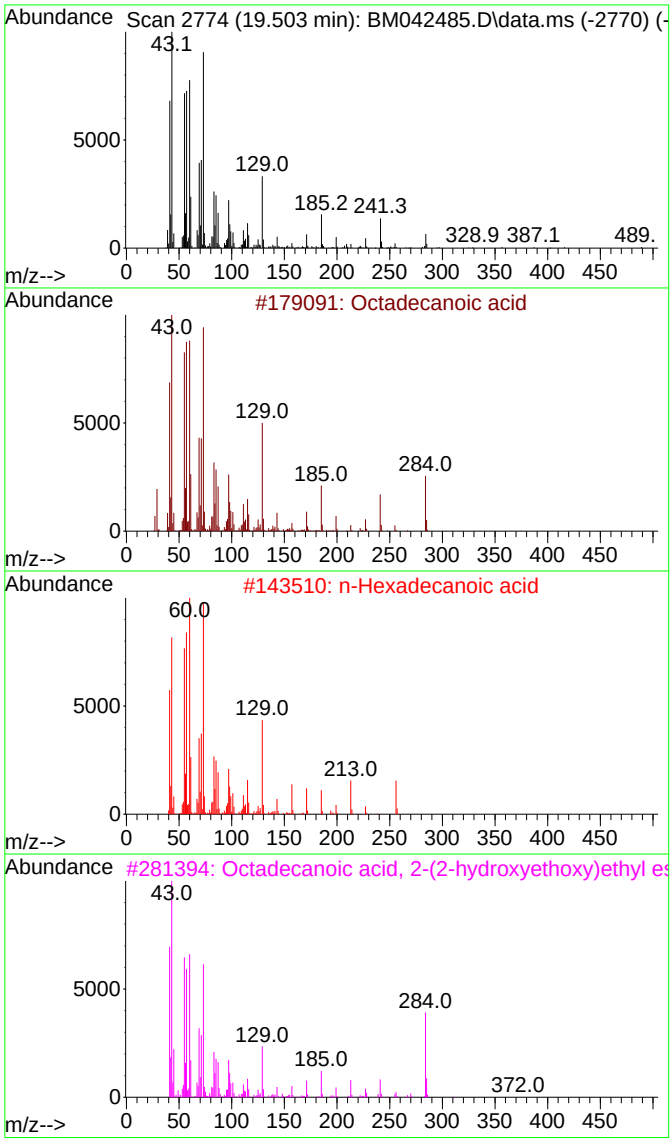
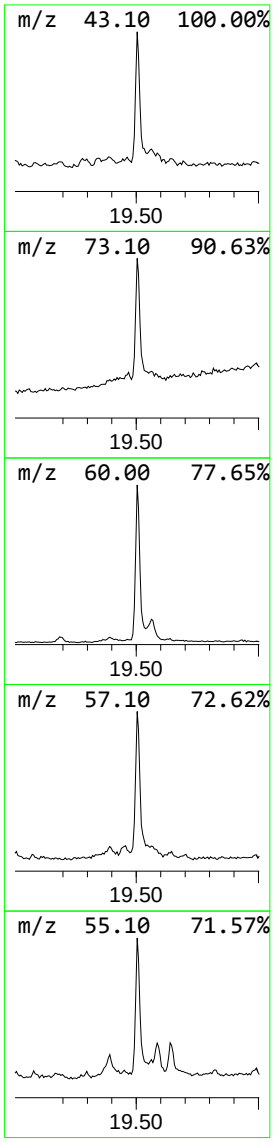
Peak Number 19 Octadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.503	10.55 ng	635579	Chrysene-d12	21.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62





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Operator : MA/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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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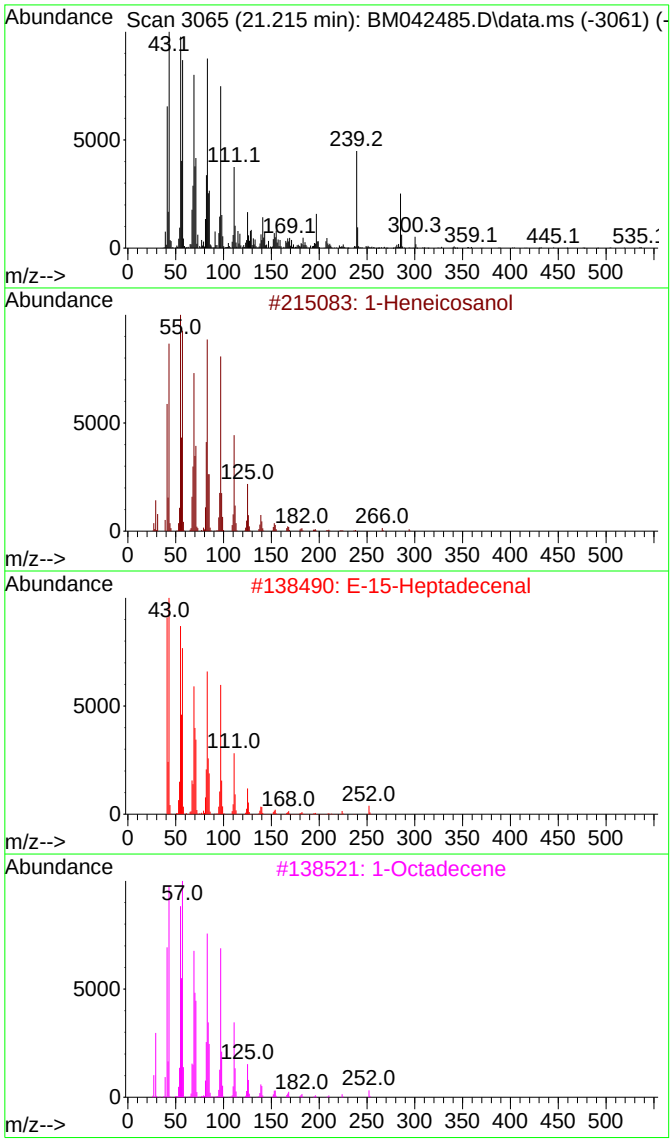
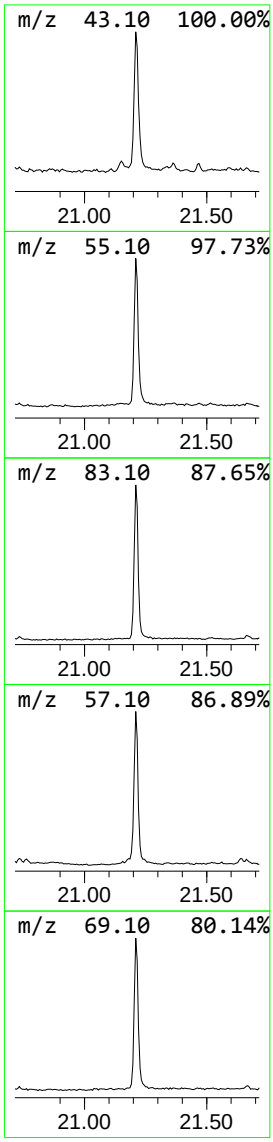
Peak Number 20 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.215	26.30 ng	1584390	Chrysene-d12	21.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
3	1-Octadecene	252	C18H36	000112-88-9	90
4	cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102723\
Data File : BM042485.D
Acq On : 27 Oct 2023 22:50
Operator : MA/JU
Sample : 04909-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LCOL-12

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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-...	5.093	9.5	ng	381979	1	7.981	803672	20.0
Ethane, 1-ethox...	7.757	50.6	ng	2032160	1	7.981	803672	20.0
unknown8.151	8.151	84.2	ng	3384140	1	7.981	803672	20.0
Triethyl phosphate	9.604	8.3	ng	542765	2	10.804	1315810	20.0
Hexanoic acid, ...	9.639	11.4	ng	746667	2	10.804	1315810	20.0
1,3-Pentanediol...	10.128	25.7	ng	1689010	2	10.804	1315810	20.0
Bicyclo[2.2.1]h...	10.228	9.8	ng	648243	2	10.804	1315810	20.0
unknown10.334	10.334	12.8	ng	840960	2	10.804	1315810	20.0
unknown11.016	11.016	8.3	ng	543880	2	10.804	1315810	20.0
unknown11.186	11.186	11.7	ng	769939	2	10.804	1315810	20.0
2-Propanol, 1-(...	11.369	11.7	ng	771850	2	10.804	1315810	20.0
unknown13.010	13.010	32.4	ng	2340470	3	14.627	1444290	20.0
1-(2-Methoxy-1-...	13.333	16.5	ng	1191870	3	14.627	1444290	20.0
2,4,7,9-Tetrame...	13.486	12.4	ng	897433	3	14.627	1444290	20.0
7-Methoxymethyl...	15.157	33.4	ng	2408810	3	14.627	1444290	20.0
n-Hexadecanoic ...	18.233	22.0	ng	1644360	4	17.380	1496070	20.0
5-Fluoro-2-meth...	18.545	74.1	ng	5544360	4	17.380	1496070	20.0
Propanoic acid,...	18.609	14.6	ng	1090840	4	17.380	1496070	20.0
Octadecanoic acid	19.503	10.6	ng	635579	5	21.556	1204650	20.0
1-Heneicosanol	21.215	26.3	ng	1584390	5	21.556	1204650	20.0