LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-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_F\Methods\8270-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140430.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	4	15	rVB	623153	707242	35.01%	3.631%
2	3.946	309	315	323	rBV	14599	23414	1.16%	0.120%
3	5.081	500	508	517	rBV	131458	192802	9.55%	0.990%
4	5.498	574	579	600	rVB	1326074	1776067	87.93%	9.120%
5	6.510	745	751	765	rBV	1461034	1924567	95.28%	9.882%
6	6.869	807	812	818	rVB	542863	700628	34.69%	3.598%
7	7.287	874	883	890	rBV7	14035	37177	1.84%	0.191%
8	7.434	897	908	916	rBV	886564	1225720	60.68%	6.294%
9	7.510	916	921	925	rVV4	18308	30925	1.53%	0.159%
10	7.681	946	950	956	rVB3	28570	46648	2.31%	0.240%
11	7.792	966	969	972	rVB3	17717	20859	1.03%	0.107%
12	7.969	995	999	1004	rVB2	18297	25000	1.24%	0.128%
13	8.022	1004	1008	1012	rBV3	16729	27518	1.36%	0.141%
14	8.151	1023	1030	1037	rBV	682015	939122	46.49%	4.822%
15	8.204	1037	1039	1043	rVV	61926	79432	3.93%	0.408%
16	8.239	1043	1045	1052	rVB7	22006	33948	1.68%	0.174%
17	8.357	1061	1065	1072	rVB5	32034	59041	2.92%	0.303%
18	8.439	1073	1079	1085	rBV4	32160	61911	3.07%	0.318%
19	8.569	1097	1101	1103	rBV	49279	60622	3.00%	0.311%
20	8.657	1112	1116	1118	rBV	19573	25070	1.24%	0.129%
21	8.692	1118	1122	1127	rVV3	23585	42335	2.10%	0.217%
22	8.739	1127	1130	1133	rVB2	16882	21745	1.08%	0.112%
23	8.834	1143	1146	1149	rVB	32405	41562	2.06%	0.213%
24	8.928	1159	1162	1165	rBV4	16666	25804	1.28%	0.132%
25	9.028	1175	1179	1181	rBV4	22081	32362	1.60%	0.166%
26	9.169	1200	1203	1207	rVB	66613	81052	4.01%	0.416%
27	9.228	1207	1213	1221	rBV	1524486	2019873	100.00%	10.371%
28	9.304	1222	1226	1230	rBV2	55248	86337	4.27%	0.443%
29	9.622	1276	1280	1287	rBV4	81840	121656	6.02%	0.625%
30	9.769	1301	1305	1309	rBV2	59227	79779	3.95%	0.410%
31	9.904	1324	1328	1332	rBV	688843	902311	44.67%	4.633%
32	9.939	1332	1334	1338	rVB	67668	68790	3.41%	0.353%
33	10.151	1367	1370	1379	rVB5	51983	97503	4.83%	0.501%
34	10.222	1379	1382	1385	rBV3	38830	55342	2.74%	0.284%
35	10.316	1394	1398	1403	rBV4	42818	90643	4.49%	0.465%
36	10.457	1418	1422	1426	rBV2	42396	61340	3.04%	0.315%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-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_F\Methods\8270-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.551	1434	1438	1444	rVB	78466	128946	6.38%	0.662%
38	10.616	1445	1449	1456	rVV	167637	232798	11.53%	1.195%
39	10.698	1458	1463	1474	rVB	808392	1078310	53.39%	5.537%
40	10.816	1479	1483	1490	rVB	143098	220191	10.90%	1.131%
41	11.286	1560	1563	1569	rVB2	95670	139783	6.92%	0.718%
42	11.398	1577	1582	1590	rBV	773304	1098052	54.36%	5.638%
43	11.469	1592	1594	1597	rVB	62010	68770	3.40%	0.353%
44	12.010	1683	1686	1694	rVB2	146825	281490	13.94%	1.445%
45	12.616	1785	1789	1792	rBV	259572	305721	15.14%	1.570%
46	12.845	1824	1828	1834	rVB	270833	392158	19.41%	2.014%
47	12.980	1846	1851	1859	rVB	1295137	1711172	84.72%	8.786%
48	14.045	2027	2032	2044	rVB2	552233	975370	48.29%	5.008%
49	15.104	2208	2212	2220	rVB	71784	147805	7.32%	0.759%
50	15.474	2271	2275	2280	rVB	87420	135616	6.71%	0.696%
51	15.539	2280	2286	2298	rVB	432413	732911	36.29%	3.763%

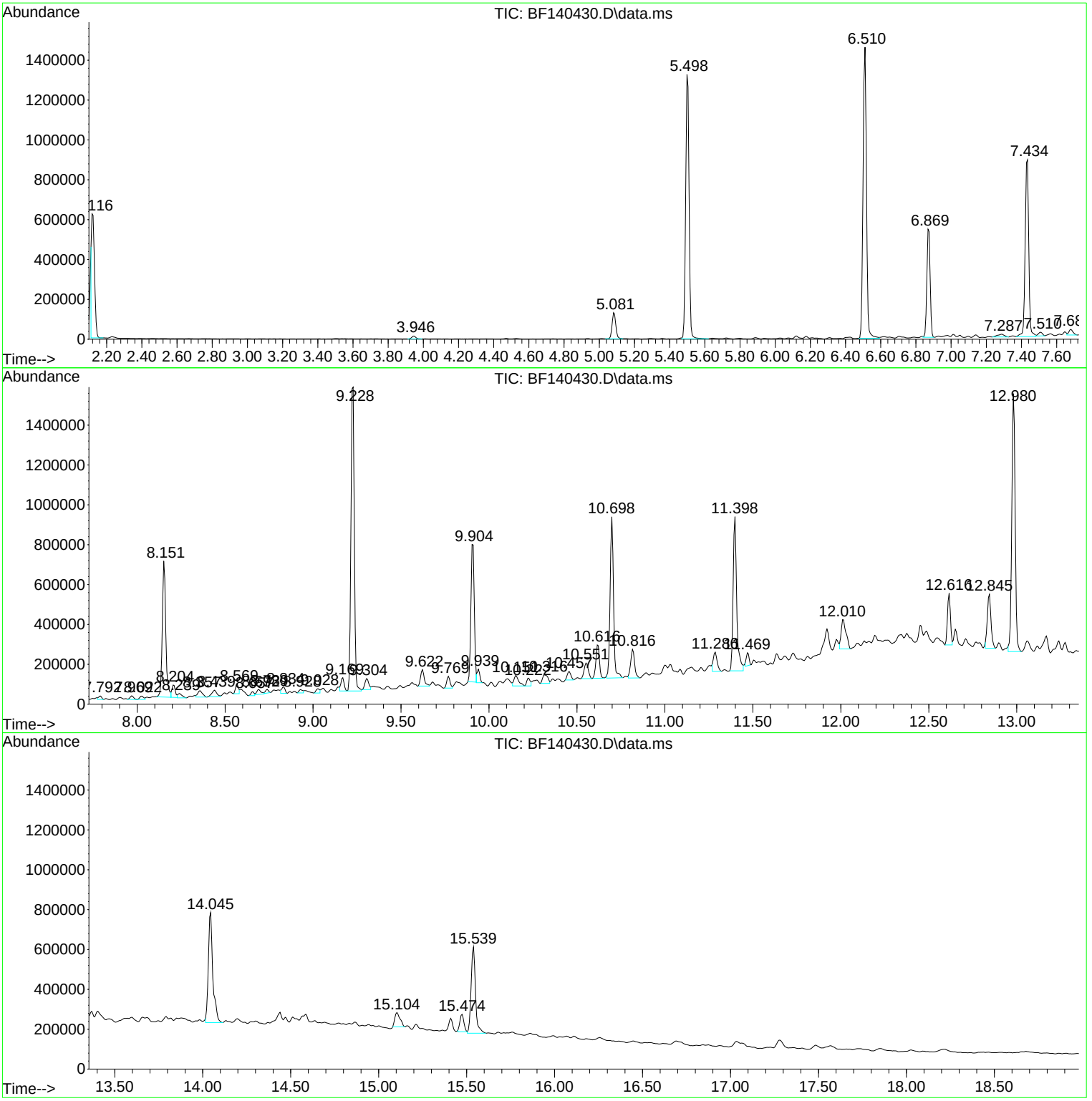
Sum of corrected areas: 19475240

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

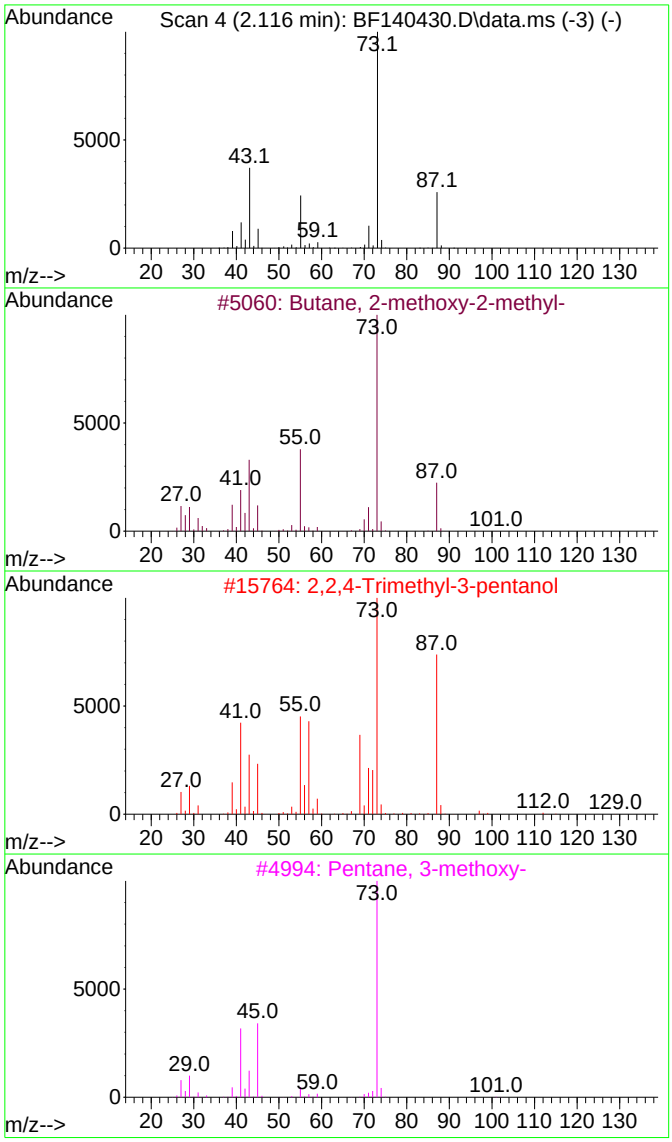
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

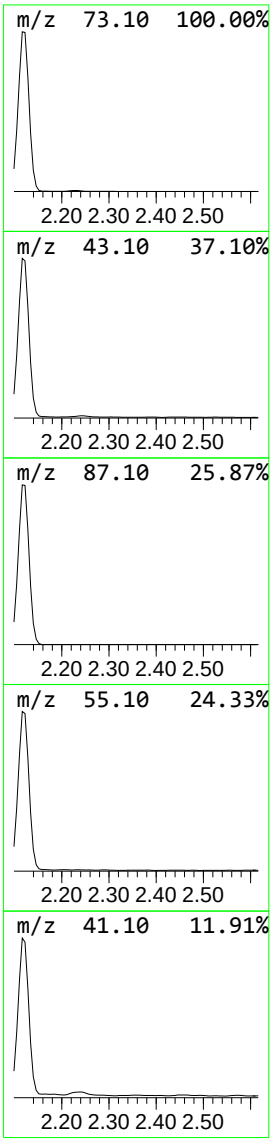
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	20.19 ng	707242	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

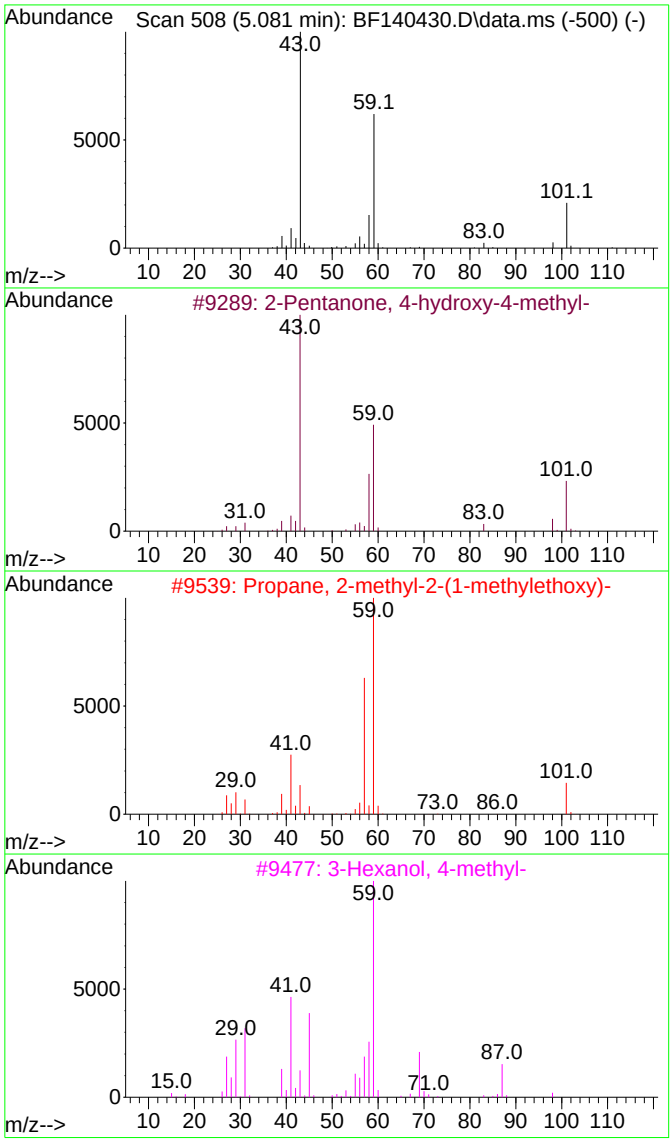
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

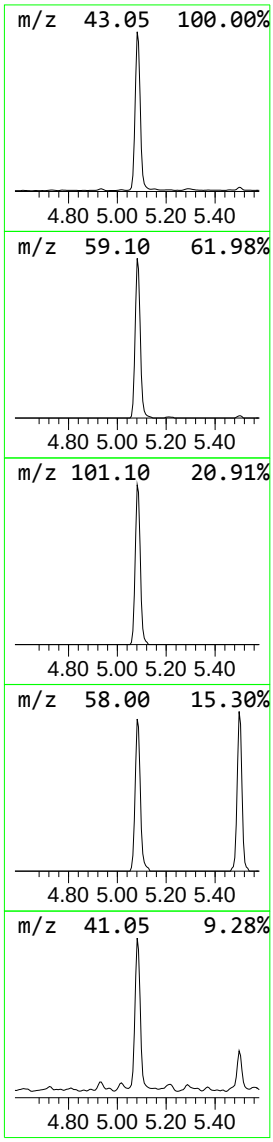
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	5.50 ng	192802	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

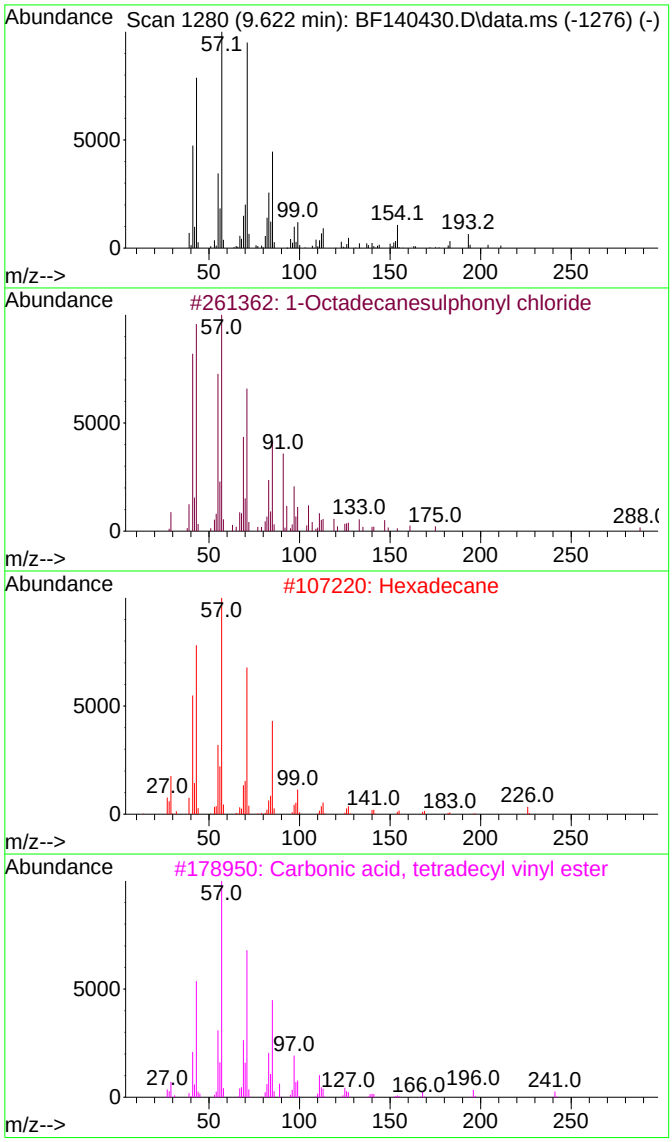
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

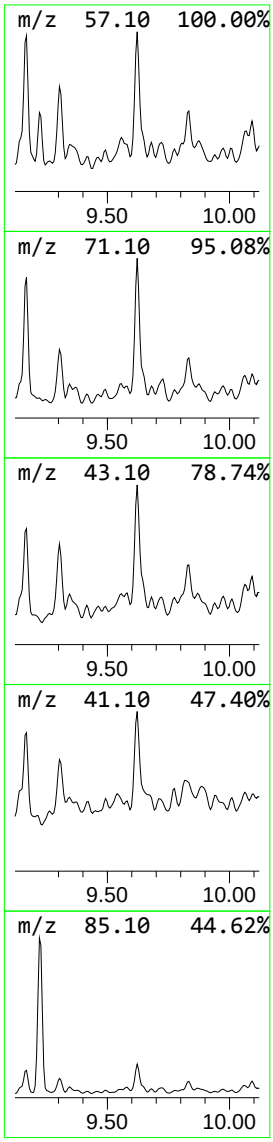
****

Peak Number 3 1-Octadecanesulphonyl chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.622	2.70 ng	121656	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	86
2	Hexadecane	226	C16H34	000544-76-3	80
3	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	78
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

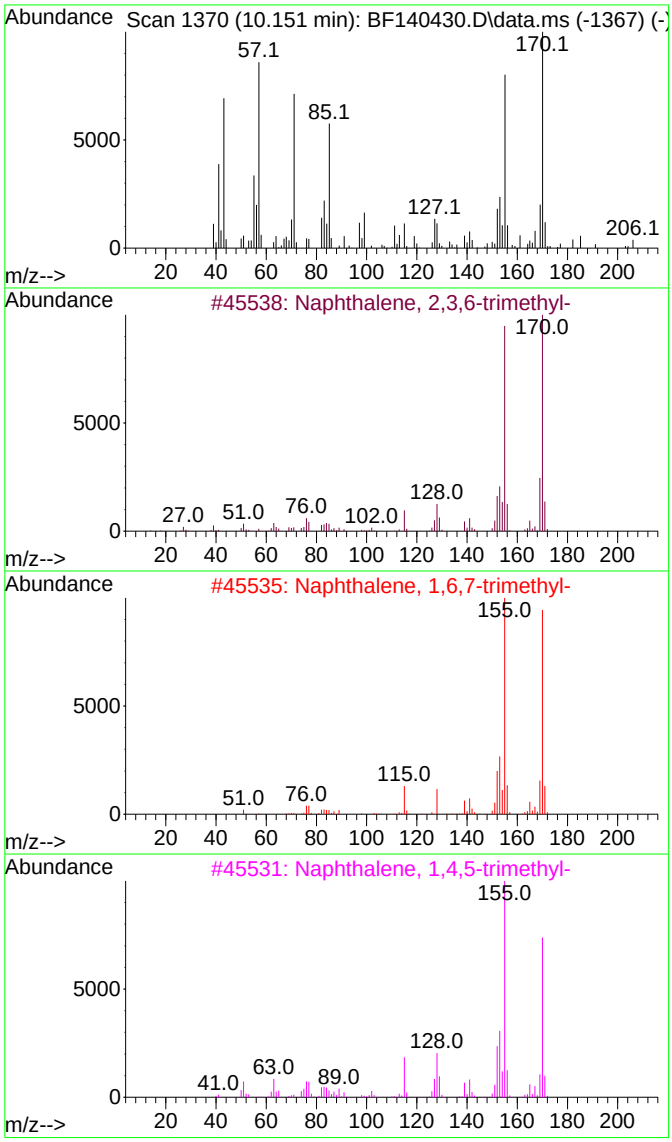
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

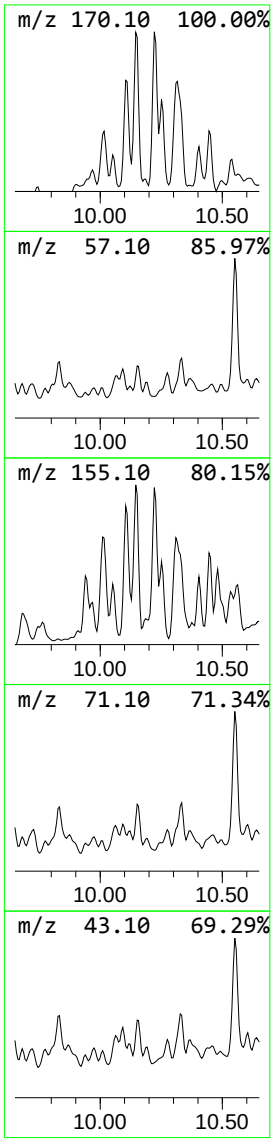
****

Peak Number 4 Naphthalene, 2,3,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.151	2.16 ng	97503	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	92
2	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	92
3	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	86
4	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	86
5	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

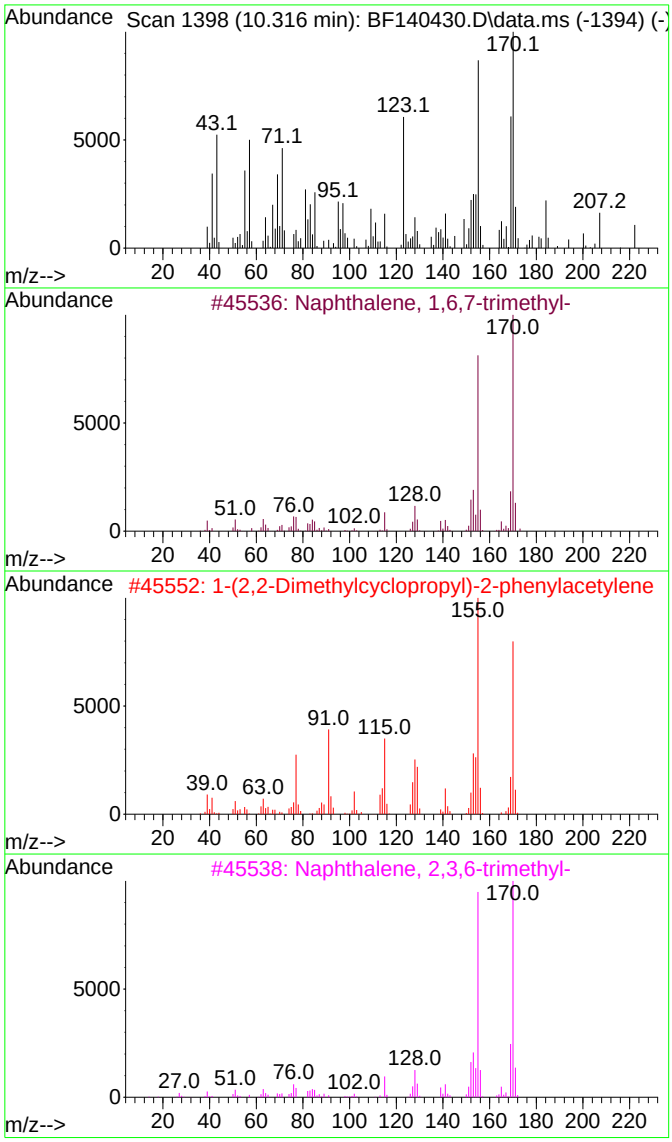
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

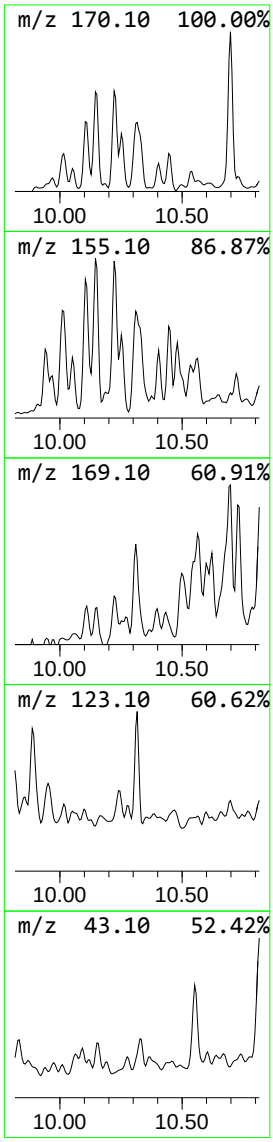
****

Peak Number 5 Naphthalene, 1,6,7-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.316	2.01 ng	90643	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	91
2	1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	64
3	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	64
4	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	64
5	1H,3H-Thieno[3,4-c]thiophene, 4,...	170	C8H10S2	015441-54-0	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

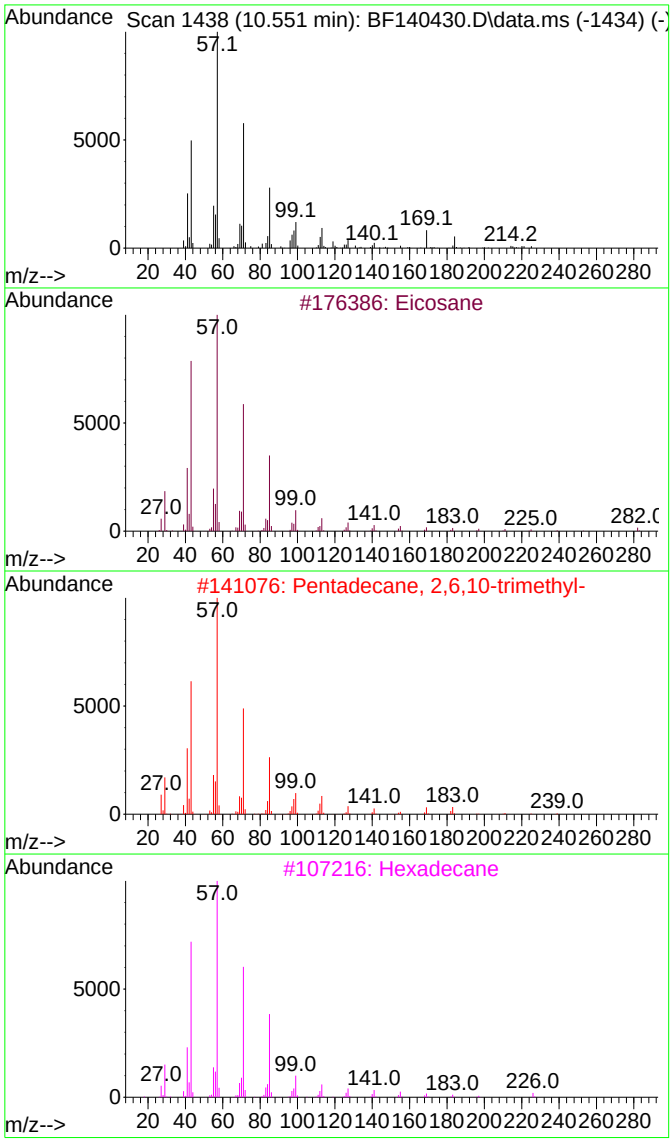
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

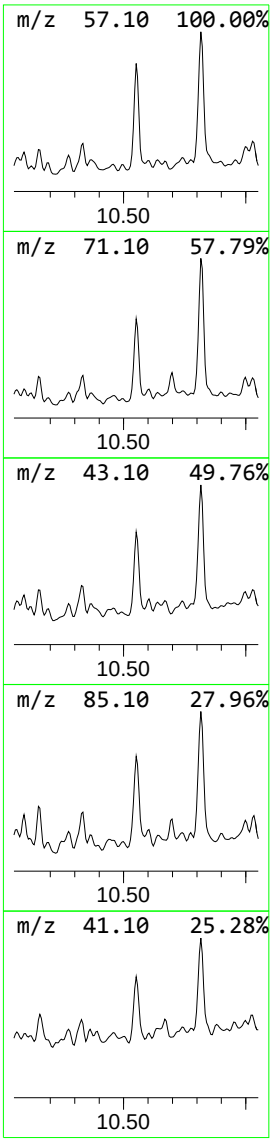
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.551	2.86 ng	128946	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3	Hexadecane	226	C16H34	000544-76-3	80
4	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	72
5	Hexacosane	366	C26H54	000630-01-3	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

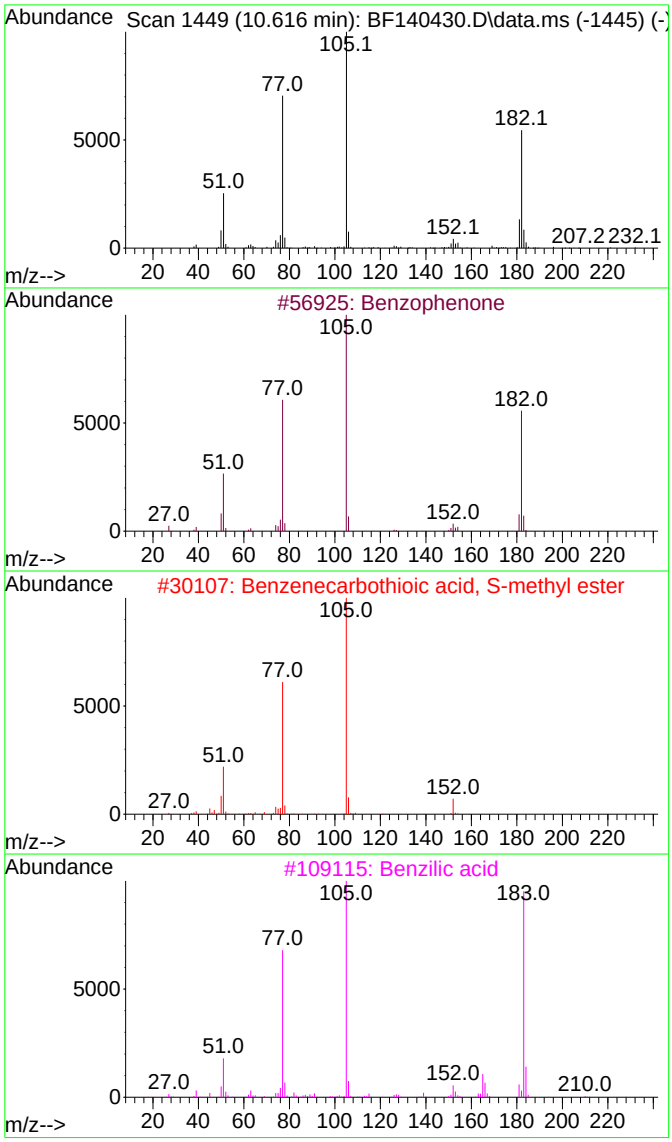
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

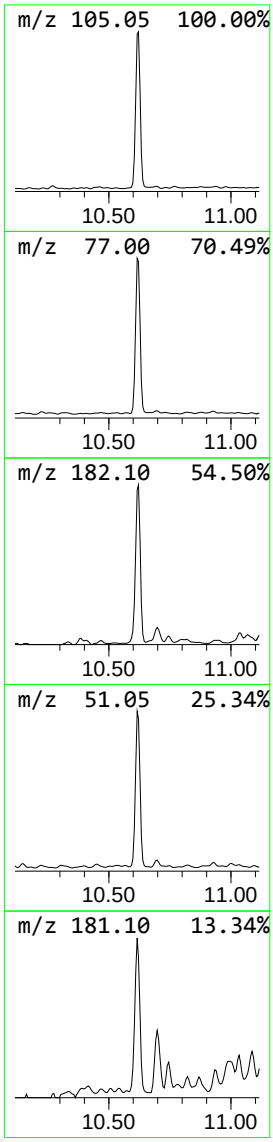
****

Peak Number 7 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	5.16 ng	232798	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3	Benzilic acid	228	C14H12O3	000076-93-7	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

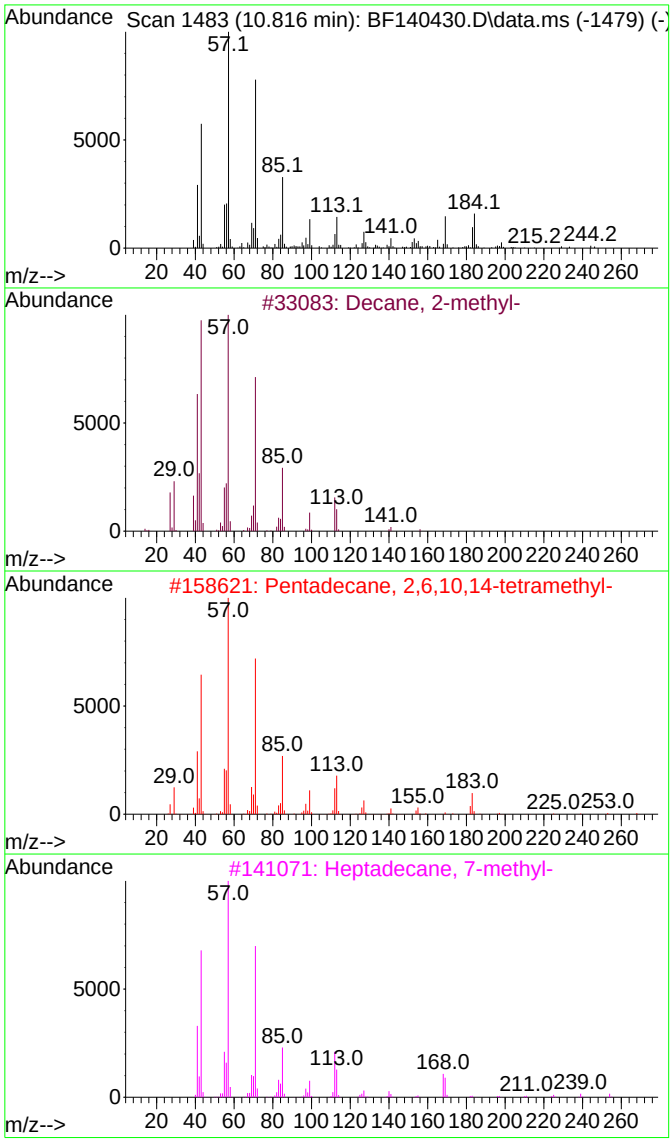
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

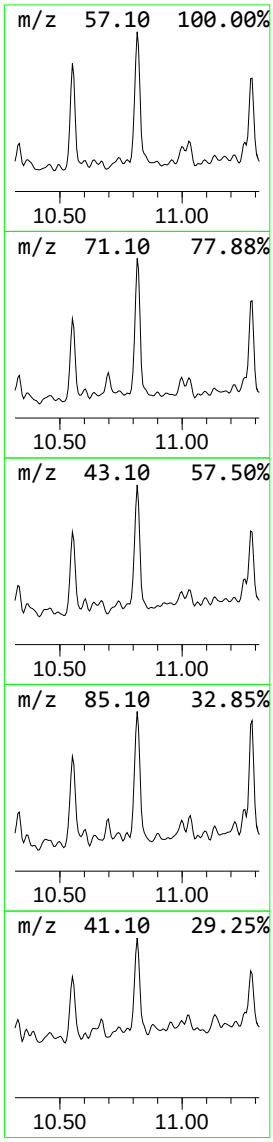
****

Peak Number 8 Decane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	4.01 ng	220191	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2-methyl-	156	C11H24	006975-98-0	81
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	80
3	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	80
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72





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Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

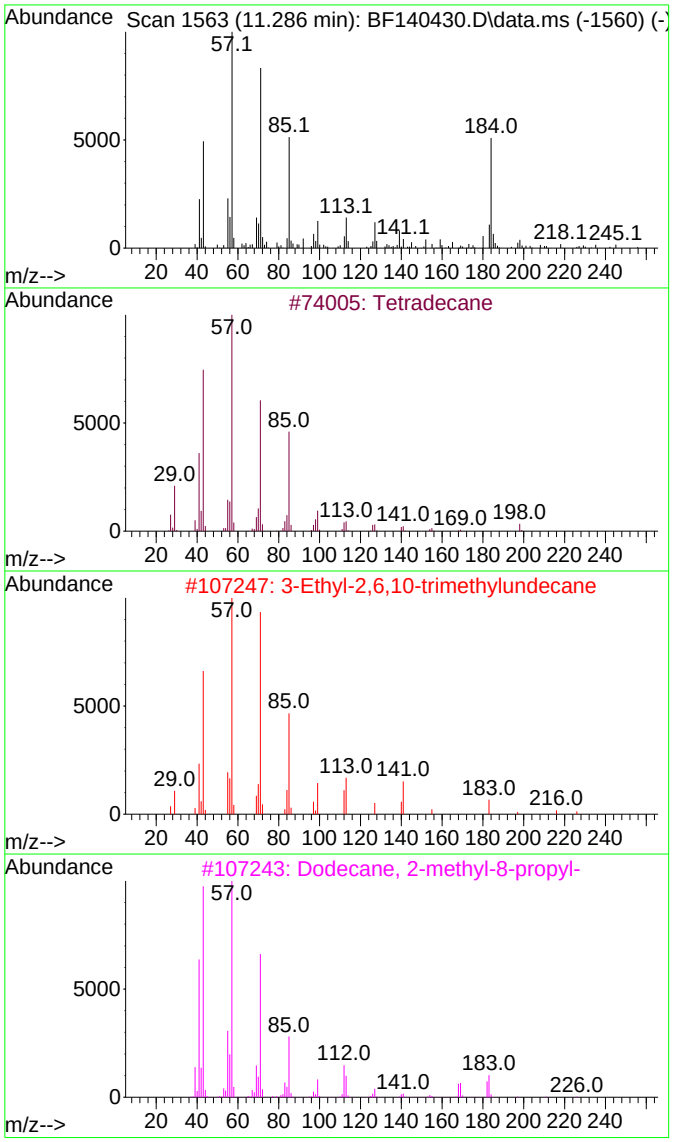
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

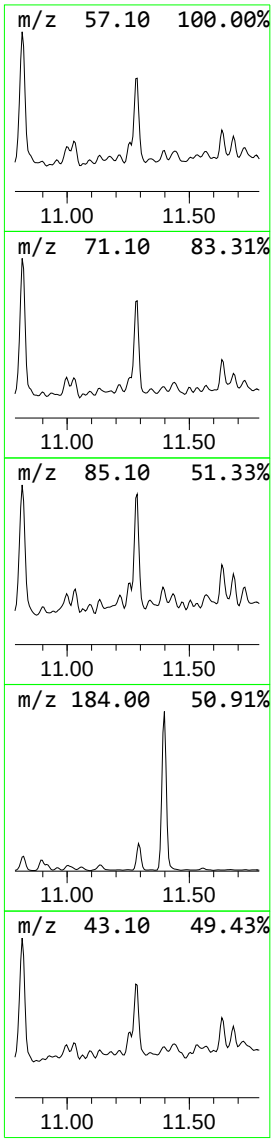
****

Peak Number 9 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.286	2.55 ng	139783	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	70
2	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	64
3	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	62
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

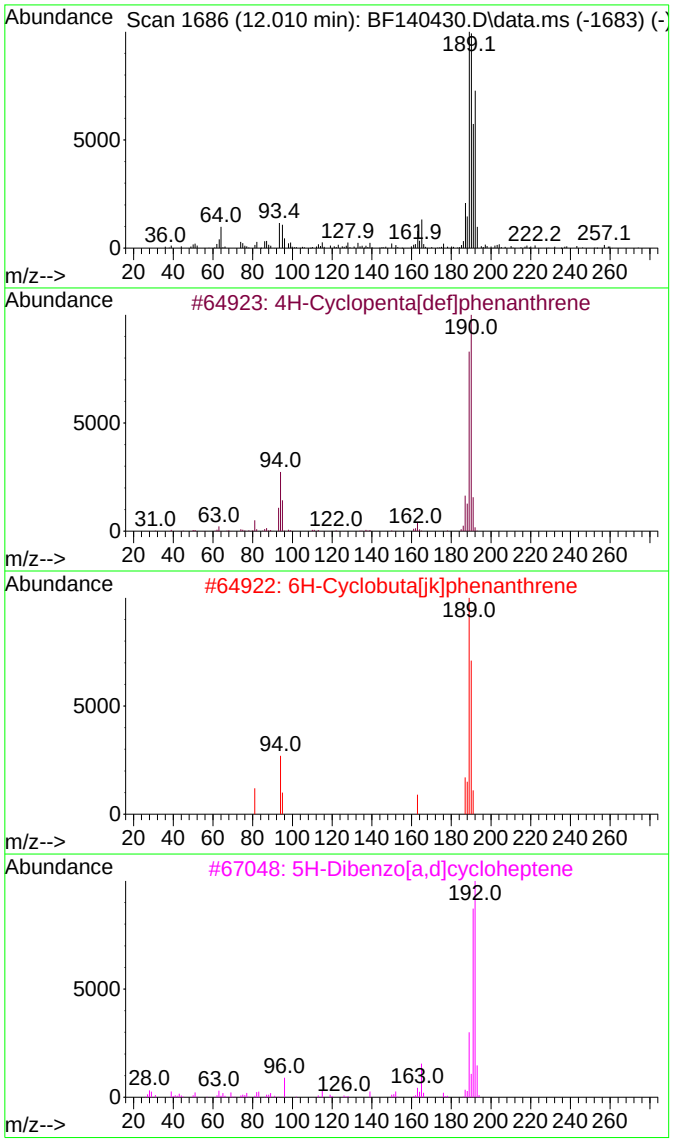
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

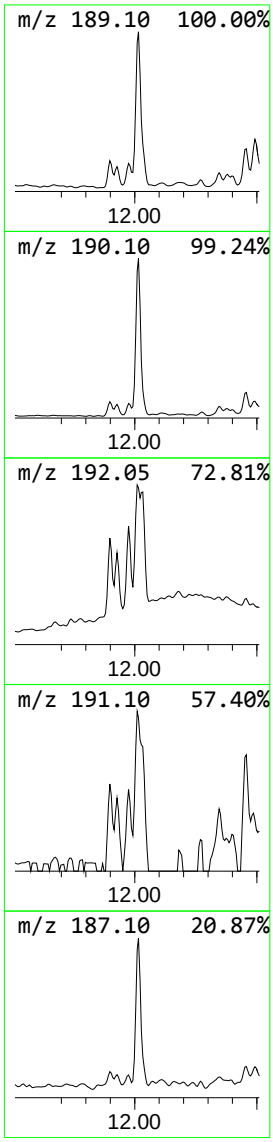
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	5.13 ng	281490	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	52
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
4	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	38
5	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111624\
Data File : BF140430.D
Acq On : 16 Nov 2024 15:23
Operator : RC/JU
Sample : P4848-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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
Butane, 2-metho...	2.116	20.2	ng	707242	1	6.875	700628	20.0
2-Pentanone, 4-...	5.081	5.5	ng	192802	1	6.875	700628	20.0
1-Octadecanesul...	9.622	2.7	ng	121656	3	9.910	902311	20.0
Naphthalene, 2,...	10.151	2.2	ng	97503	3	9.910	902311	20.0
Naphthalene, 1,...	10.316	2.0	ng	90643	3	9.910	902311	20.0
Eicosane	10.551	2.9	ng	128946	3	9.910	902311	20.0
Benzophenone	10.616	5.2	ng	232798	3	9.910	902311	20.0
Decane, 2-methyl-	10.816	4.0	ng	220191	4	11.398	1098050	20.0
Tetradecane	11.286	2.5	ng	139783	4	11.398	1098050	20.0
4H-Cyclopenta[d...	12.010	5.1	ng	281490	4	11.398	1098050	20.0