LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	6	13	25	rVB	360284	575072	43.31%	5.088%
2	5.104	506	512	517	rBV	30018	42816	3.22%	0.379%
3	5.498	574	579	585	rBV	861664	1152982	86.83%	10.200%
4	5.622	596	600	607	rBV	13460	20972	1.58%	0.186%
5	5.992	658	663	673	rVB	42412	62325	4.69%	0.551%
6	6.128	677	686	691	rBV3	10769	22460	1.69%	0.199%
7	6.269	706	710	711	rBV	18575	20654	1.56%	0.183%
8	6.287	711	713	718	rVB	24520	30023	2.26%	0.266%
9	6.504	744	750	755	rBV	862116	1137358	85.65%	10.062%
10	6.557	756	759	764	rVB	12887	15644	1.18%	0.138%
11	6.887	810	815	820	rBV	369211	453679	34.17%	4.014%
12	7.263	874	879	889	rBV	10631	17135	1.29%	0.152%
13	7.445	904	910	915	rBV	614338	761360	57.34%	6.736%
14	7.698	948	953	958	rBV	36644	43233	3.26%	0.382%
15	7.998	992	1004	1007	rBV4	8813	14766	1.11%	0.131%
16	8.169	1028	1033	1038	rBV	471311	575472	43.34%	5.091%
17	8.381	1065	1069	1073	rBV2	13961	17116	1.29%	0.151%
18	8.592	1101	1105	1112	rBV2	9712	17532	1.32%	0.155%
19	9.245	1210	1216	1226	rBV	998204	1327884	100.00%	11.748%
20	9.692	1285	1292	1295	rBV4	7321	14736	1.11%	0.130%
21	9.733	1295	1299	1315	rVB4	17100	35403	2.67%	0.313%
22	9.922	1325	1331	1343	rVB	497420	636551	47.94%	5.632%
23	10.051	1349	1353	1360	rBV	30601	41548	3.13%	0.368%
24	10.410	1410	1414	1421	rBV2	13110	18204	1.37%	0.161%
25	10.633	1447	1452	1460	rVB	314913	389111	29.30%	3.442%
26	10.710	1460	1465	1479	rBV	570299	741606	55.85%	6.561%
27	10.945	1494	1505	1509	rBV	51186	68749	5.18%	0.608%
28	11.069	1521	1526	1530	rBV2	10390	13852	1.04%	0.123%
29	11.316	1564	1568	1573	rVB5	10927	15444	1.16%	0.137%
30	11.410	1579	1584	1589	rBV	441703	542404	40.85%	4.799%
31	11.645	1620	1624	1630	rBV4	5625	13619	1.03%	0.120%
32	11.857	1656	1660	1668	rBV4	10725	16501	1.24%	0.146%
33	11.933	1668	1673	1683	rBV	163293	242755	18.28%	2.148%
34	12.433	1754	1758	1765	rVB	13479	19602	1.48%	0.173%
35	12.627	1785	1791	1802	rBV3	88462	210532	15.85%	1.863%
36	12.716	1802	1806	1819	rVB	35414	63294	4.77%	0.560%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.992	1848	1853	1858	rBV	646611	802684	60.45%	7.101%
38	13.568	1947	1951	1964	rVB6	9067	19273	1.45%	0.171%
39	13.898	2002	2007	2021	rBV	37010	83574	6.29%	0.739%
40	14.045	2027	2032	2040	rBV	292364	374203	28.18%	3.311%
41	14.515	2109	2112	2119	rBV2	8058	13509	1.02%	0.120%
42	14.674	2136	2139	2148	rVB	14634	21050	1.59%	0.186%
43	14.904	2174	2178	2185	rVB	64180	85126	6.41%	0.753%
44	15.527	2277	2284	2294	rBV	282093	449723	33.87%	3.979%
45	16.004	2361	2365	2371	rBV2	10143	17970	1.35%	0.159%
46	16.527	2451	2454	2467	rVB6	8628	18933	1.43%	0.168%
47	18.245	2739	2746	2753	rVB4	9436	24785	1.87%	0.219%

Sum of corrected areas: 11303224

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
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Operator : RC/JU
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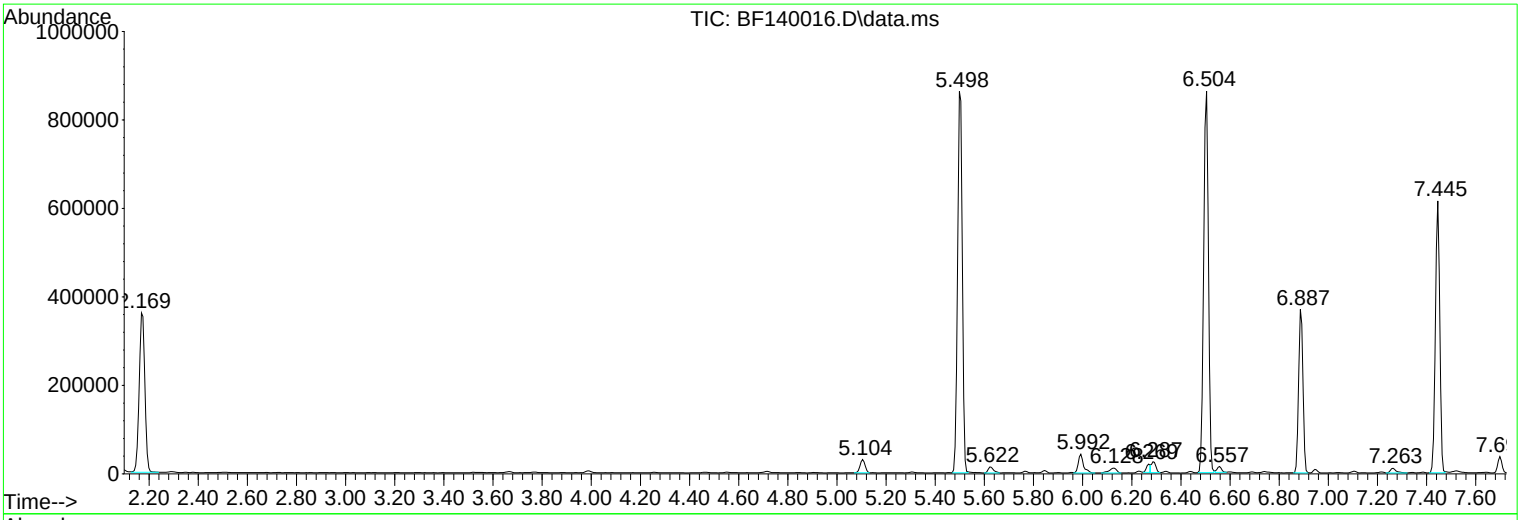
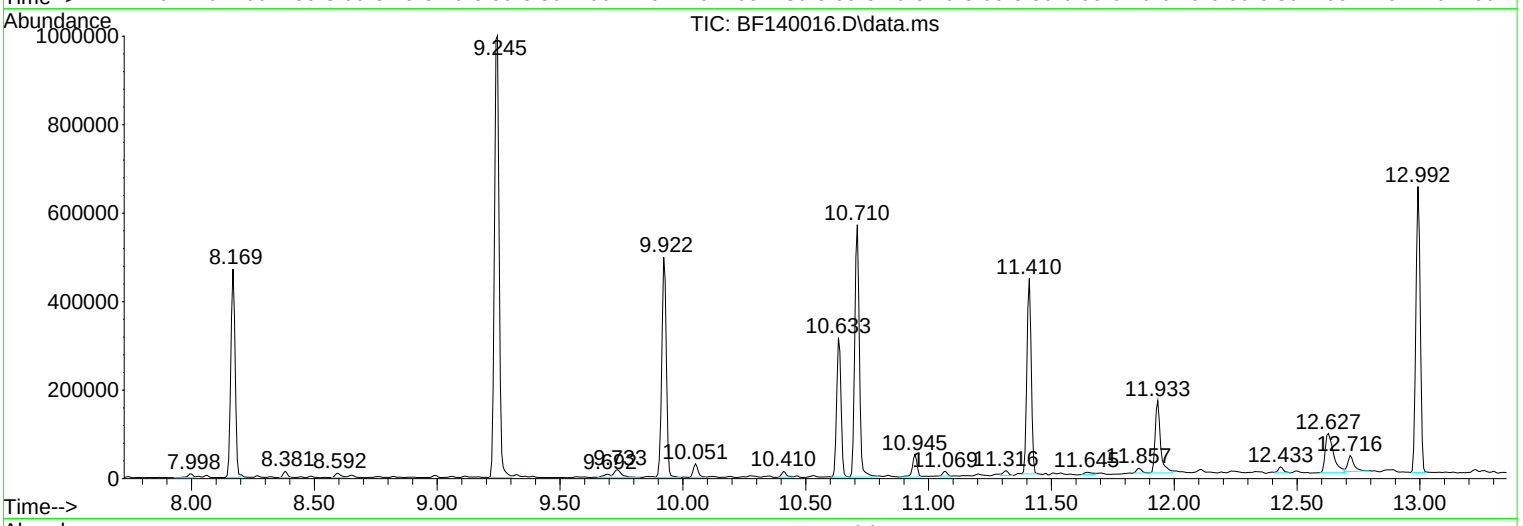
Misc :
ALS Vial : 17 Sample Multiplier: 1

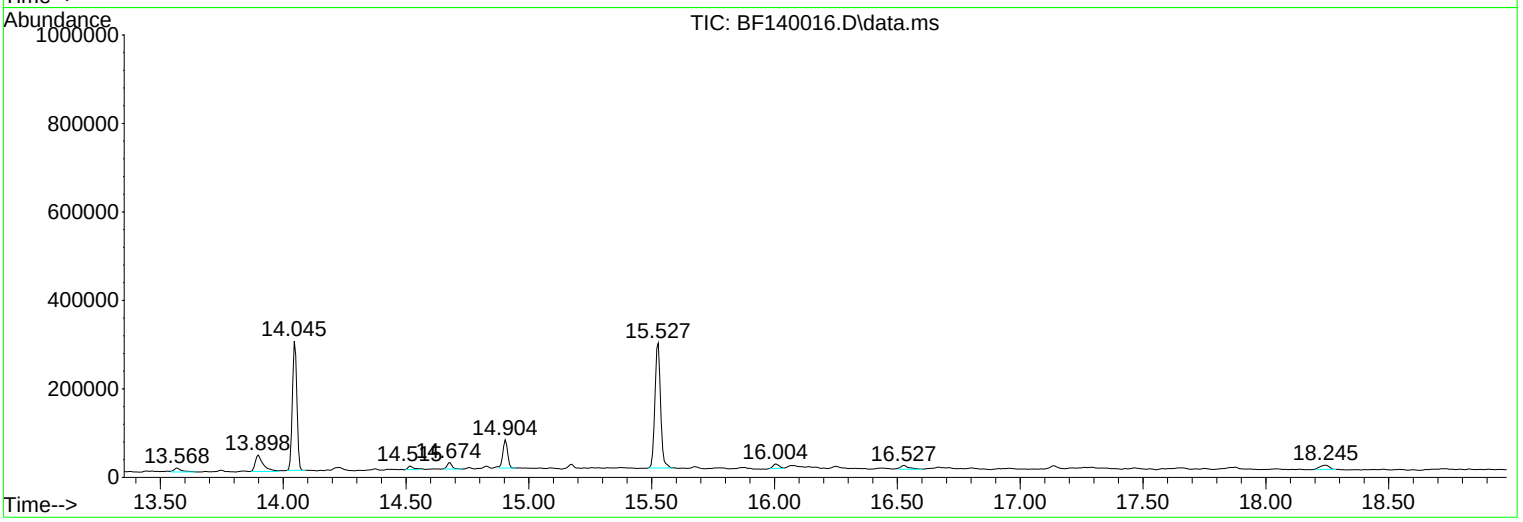
Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
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Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

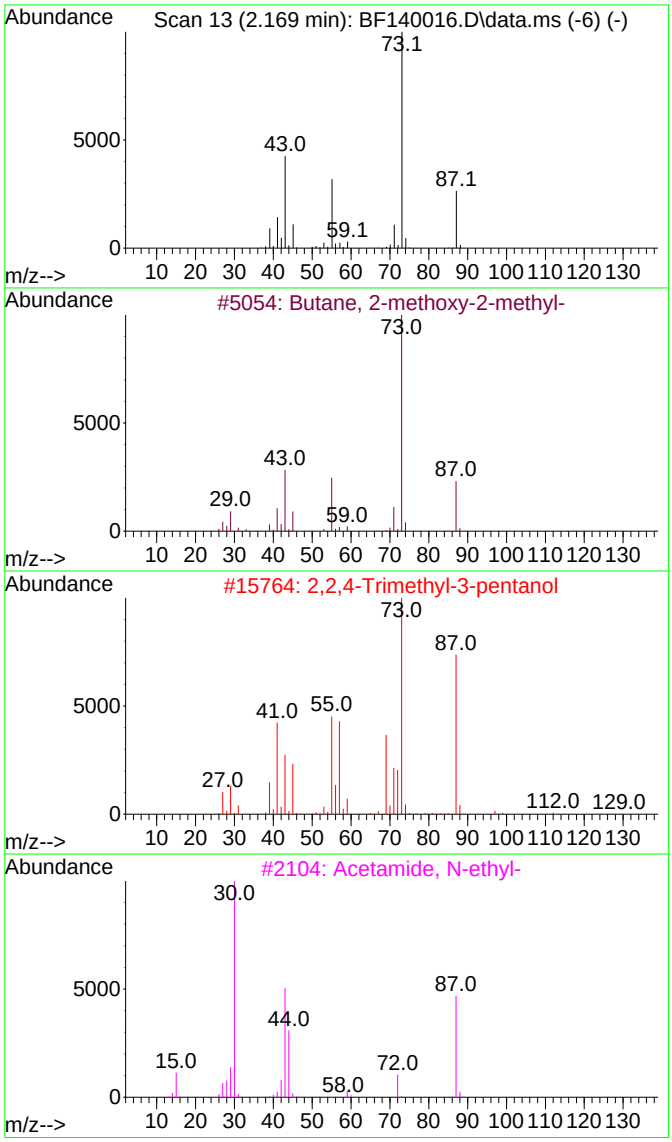
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

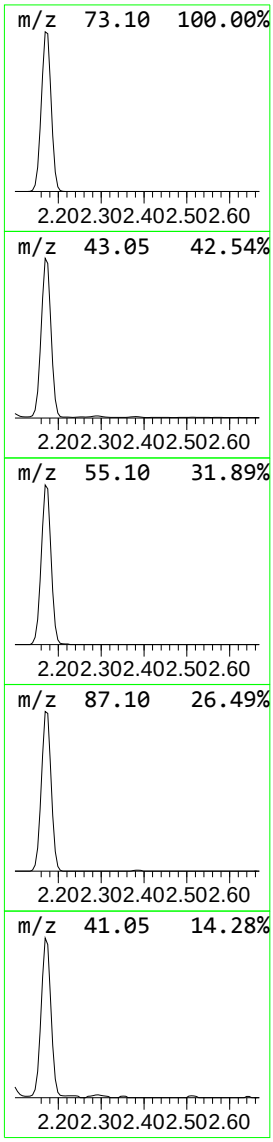
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	25.35 ng	575072	1,4-Dichlorobenzene-d4	6.887

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	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

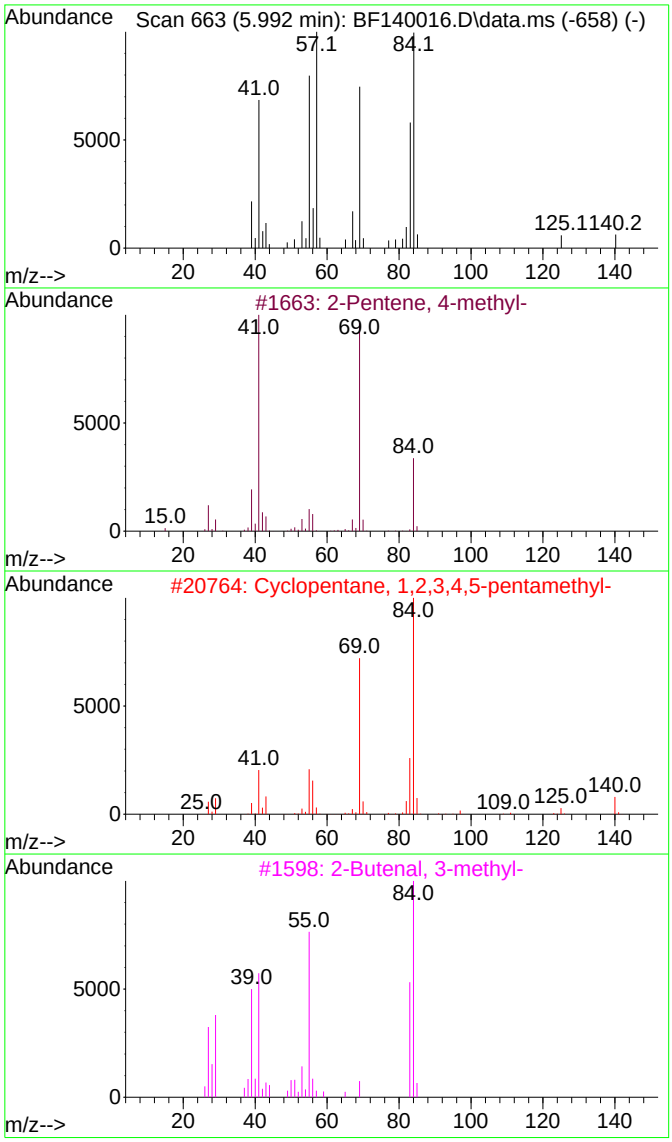
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

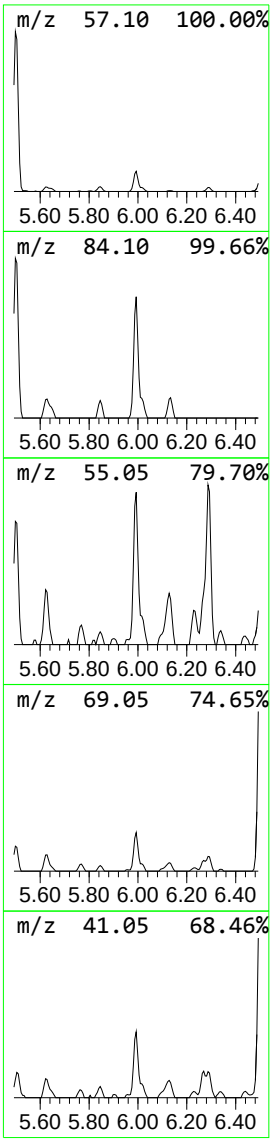
****

Peak Number 2 unknown5.992 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.992	2.75 ng	62325	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4-methyl-	84	C6H12	004461-48-7	47
2	Cyclopentane, 1,2,3,4,5-pentamet...	140	C10H20	1000152-79-7	46
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	46
4	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	43
5	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

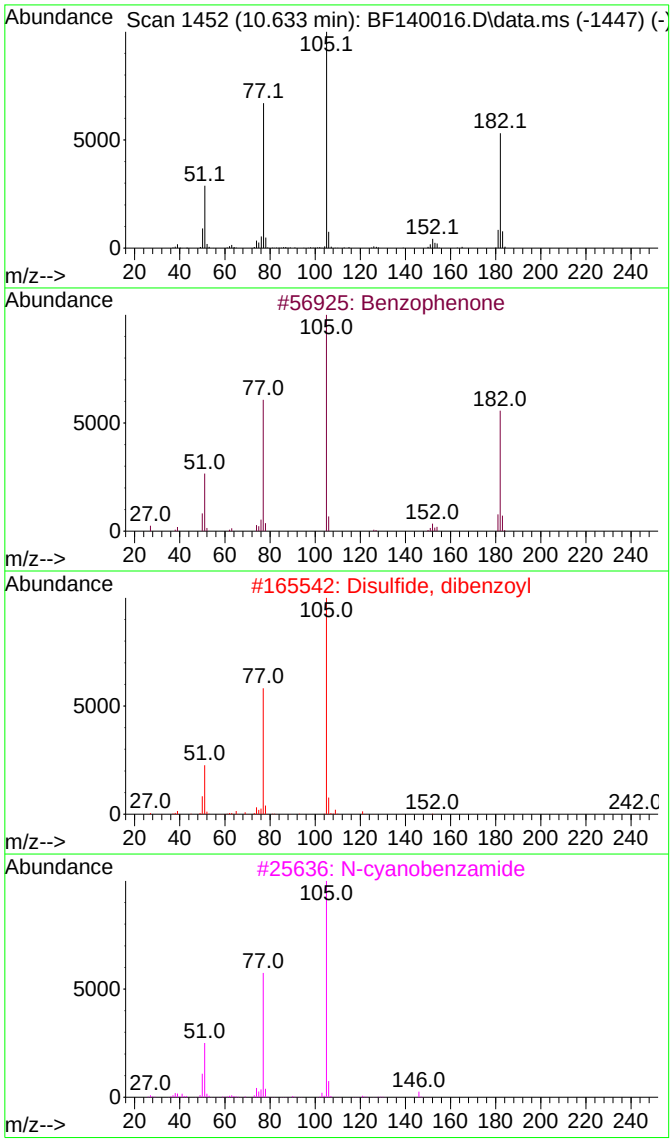
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

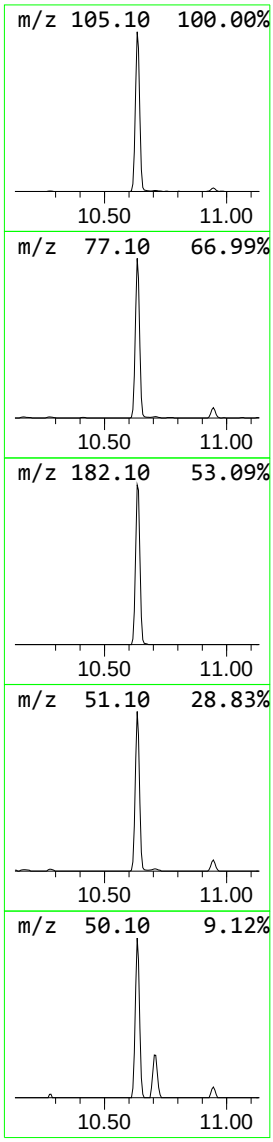
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	12.23 ng	389111	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	52
3	N-cyanobenzamide	146	C8H6N2O	015150-25-1	50
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50
5	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

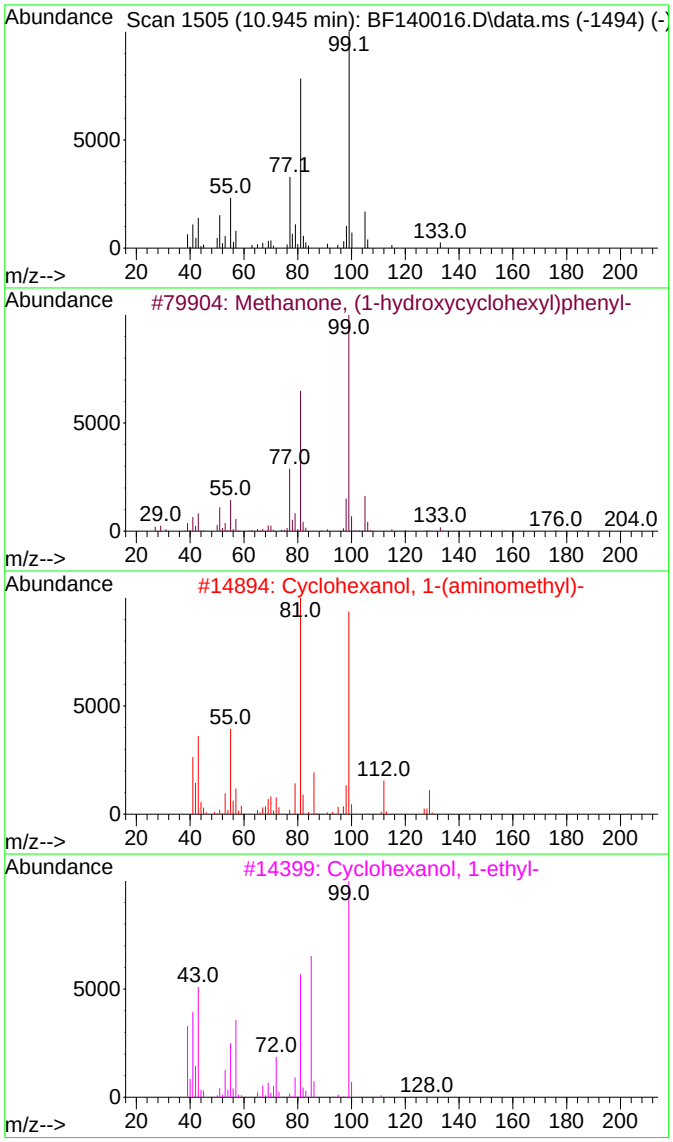
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

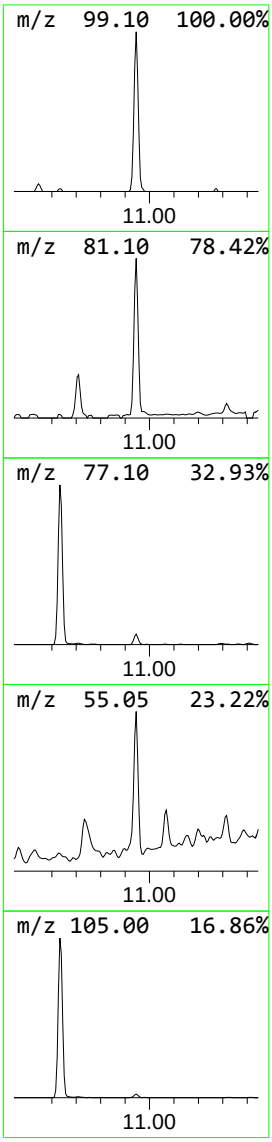
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	2.53 ng	68749	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	90
2	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
3	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	38
4	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	38
5	2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

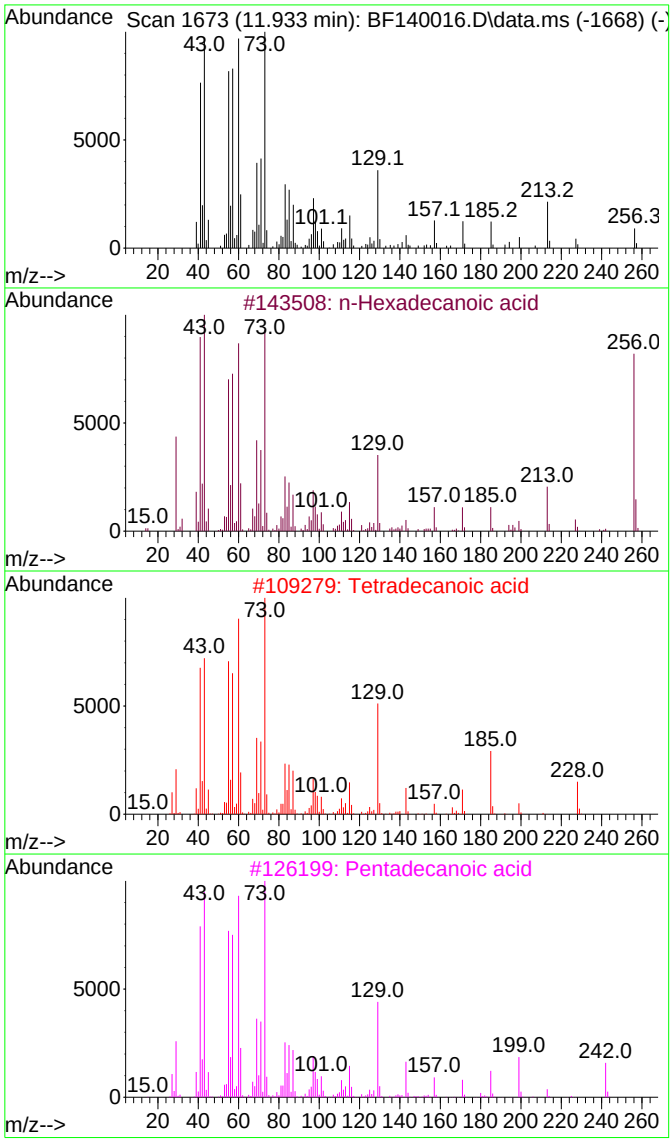
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

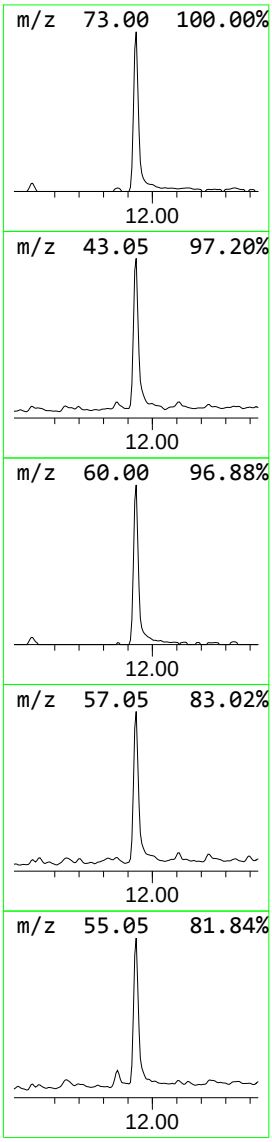
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	8.95 ng	242755	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Operator : RC/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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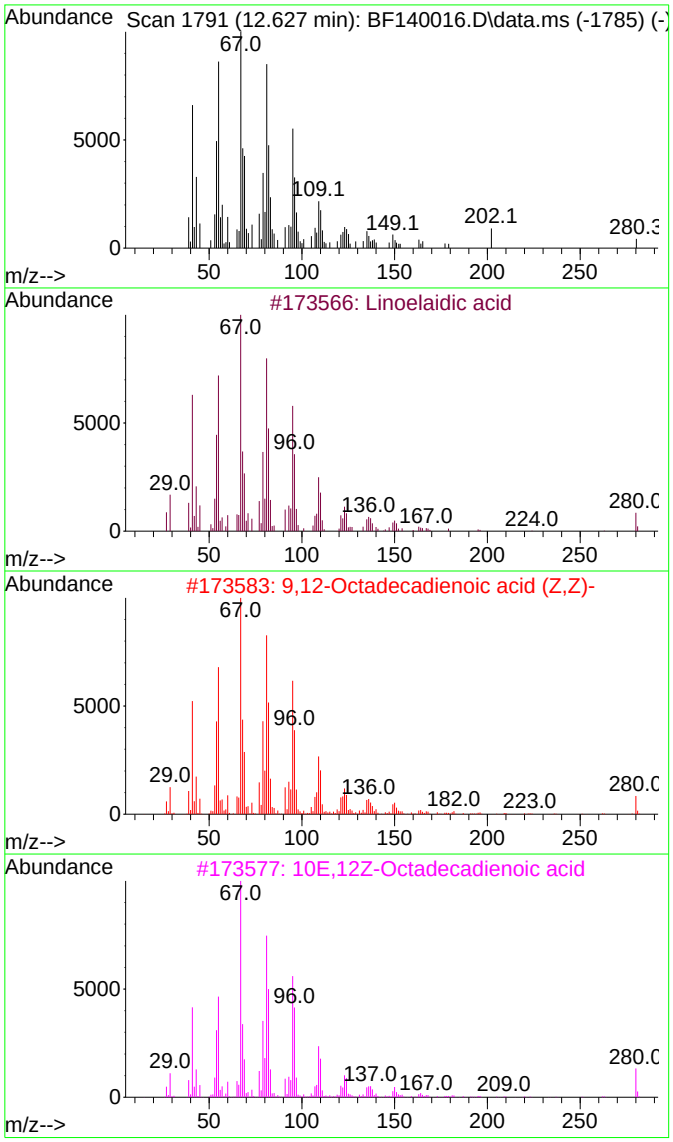
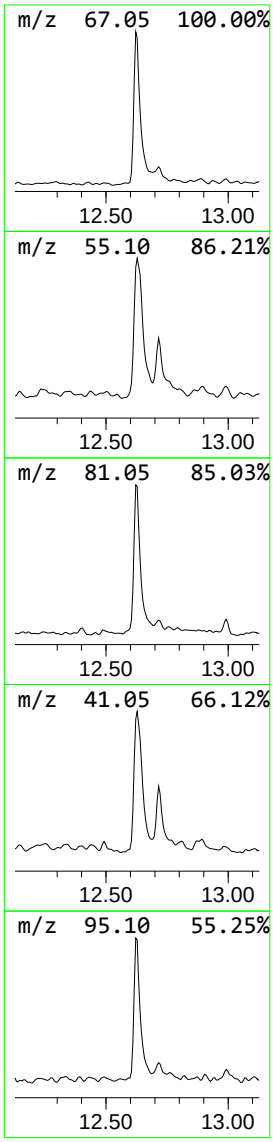
Peak Number 6 Linoelaidic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	7.76 ng	210532	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Linoelaidic acid	280	C18H32O2	000506-21-8	99
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
3	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	96
4	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	93
5	1-Hexadecyne	222	C16H30	000629-74-3	91





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Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

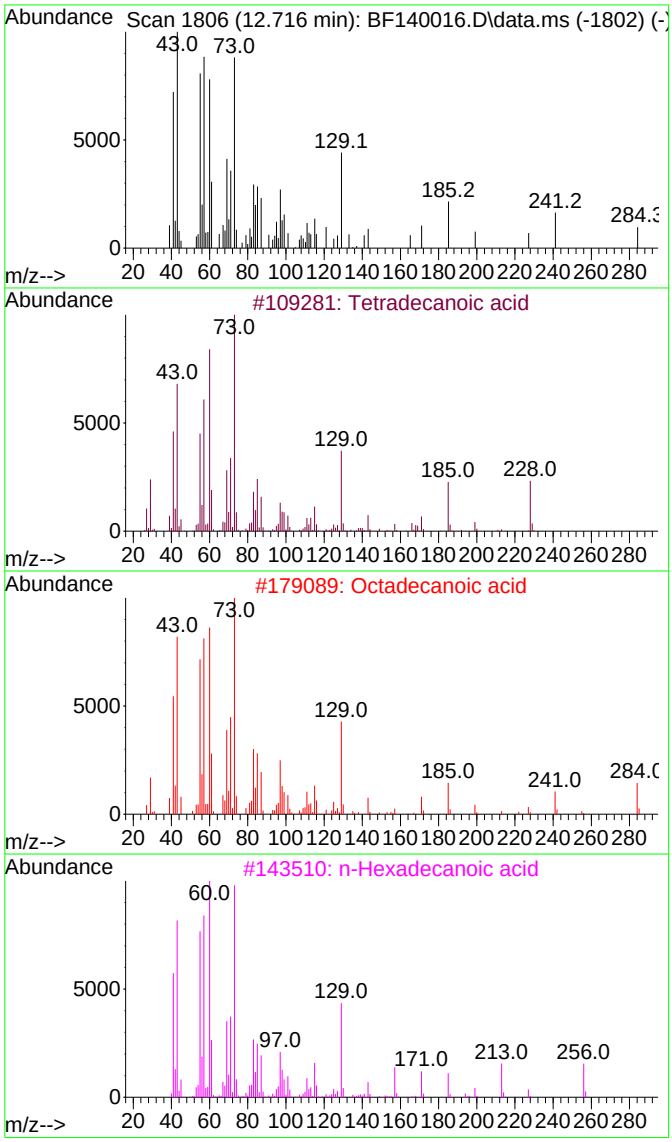
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

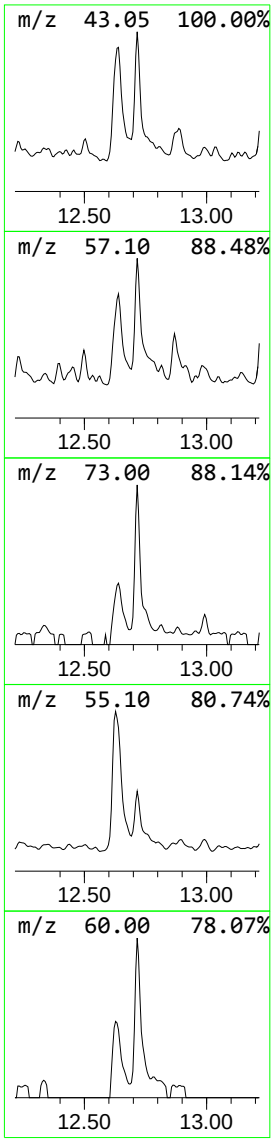
****

Peak Number 7 Tetradecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.33 ng	63294	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	Octadecanoic acid	284	C18H36O2	000057-11-4	52
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

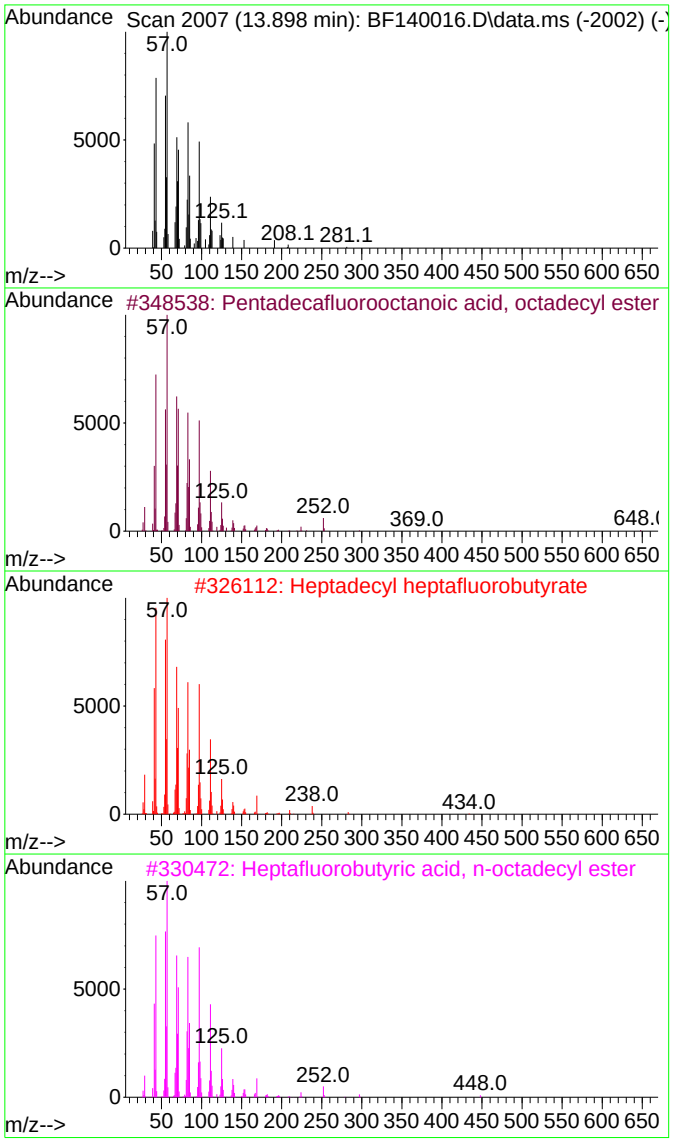
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

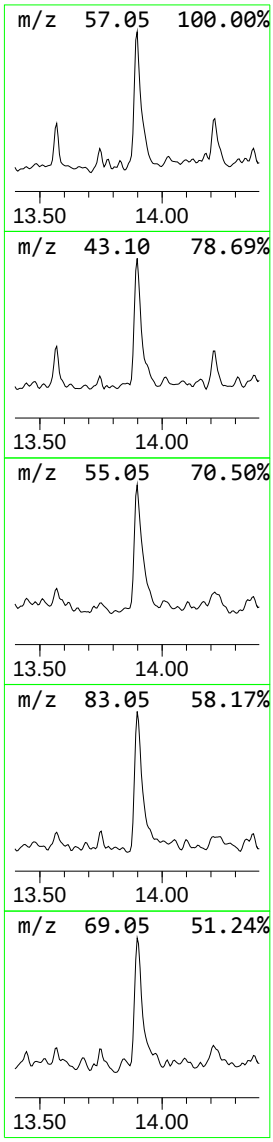
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.47 ng	83574	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

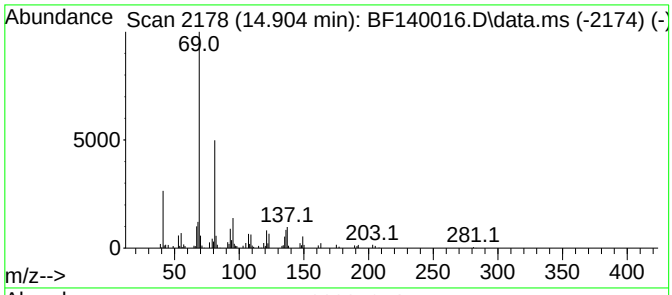
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

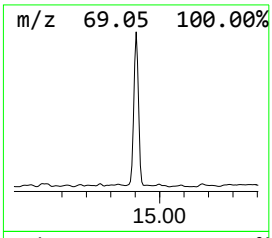
****

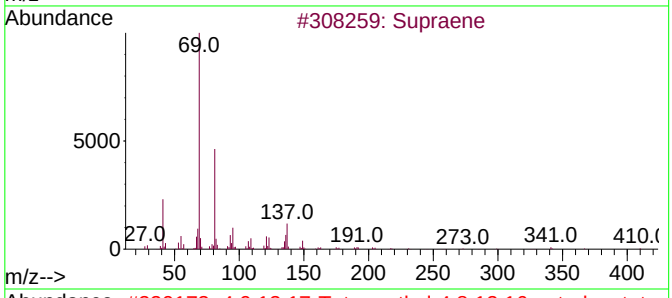
Peak Number 9 Supraene Concentration Rank 6

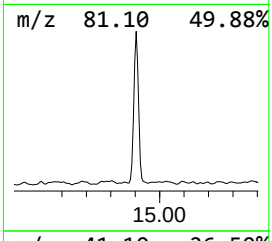
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	3.79 ng	85126	Perylene-d12	15.527

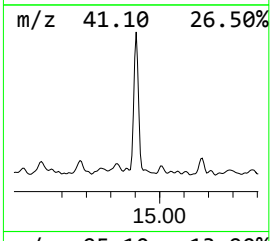
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72

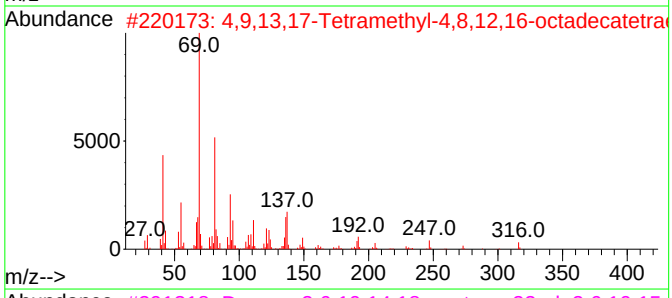


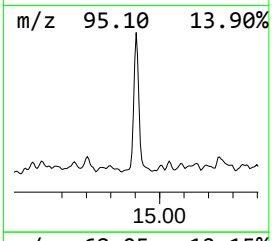


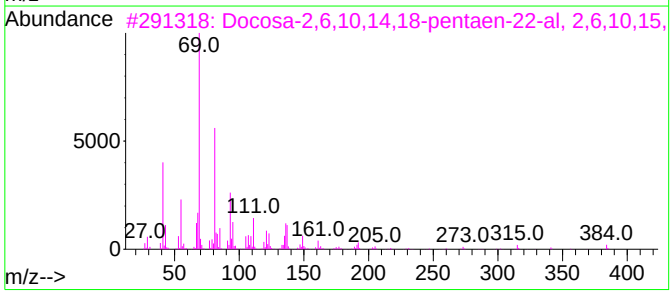


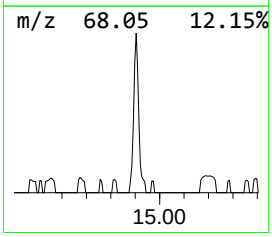












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102424\
Data File : BF140016.D
Acq On : 24 Oct 2024 22:29
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.169	25.4	ng	575072	1	6.887	453679	20.0
unknown5.992	5.992	2.8	ng	62325	1	6.887	453679	20.0
Benzophenone	10.633	12.2	ng	389111	3	9.922	636551	20.0
Methanone, (1-h...	10.945	2.5	ng	68749	4	11.410	542404	20.0
n-Hexadecanoic ...	11.933	8.9	ng	242755	4	11.410	542404	20.0
Linoelaidic acid	12.627	7.8	ng	210532	4	11.410	542404	20.0
Tetradecanoic acid	12.716	2.3	ng	63294	4	11.410	542404	20.0
Pentadecafluoro...	13.898	4.5	ng	83574	5	14.045	374203	20.0
Supraene	14.904	3.8	ng	85126	6	15.527	449723	20.0