LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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: BF140042.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.164	5	12	19	rVB	417434	656746	40.75%	4.734%
2	5.104	506	512	517	rBV	35183	50690	3.15%	0.365%
3	5.499	573	579	585	rBV	1022129	1325411	82.24%	9.554%
4	5.622	595	600	608	rVB	15846	24411	1.51%	0.176%
5	5.993	658	663	671	rVB	45585	68085	4.22%	0.491%
6	6.122	676	685	699	rBV3	12882	28448	1.77%	0.205%
7	6.269	706	710	711	rBV	19273	23275	1.44%	0.168%
8	6.287	711	713	718	rVB	27126	31740	1.97%	0.229%
9	6.504	744	750	755	rBV	997395	1318608	81.82%	9.505%
10	6.551	755	758	765	rVB2	17487	24640	1.53%	0.178%
11	6.887	810	815	820	rBV	435692	524205	32.53%	3.779%
12	7.263	875	879	889	rVB2	12399	20403	1.27%	0.147%
13	7.446	904	910	915	rBV	708160	894679	55.51%	6.449%
14	7.698	948	953	958	rBV	43203	51178	3.18%	0.369%
15	8.169	1027	1033	1038	rBV	555216	687265	42.64%	4.954%
16	8.381	1065	1069	1074	rVB	18112	22436	1.39%	0.162%
17	8.592	1101	1105	1111	rBV	12135	19638	1.22%	0.142%
18	9.239	1210	1215	1226	rBV	1209883	1611652	100.00%	11.618%
19	9.692	1285	1292	1295	rBV5	8595	18019	1.12%	0.130%
20	9.734	1295	1299	1312	rVB4	20731	44799	2.78%	0.323%
21	9.922	1325	1331	1342	rVB	627387	803468	49.85%	5.792%
22	10.051	1349	1353	1361	rBV	33435	48352	3.00%	0.349%
23	10.410	1409	1414	1420	rBV	20694	29475	1.83%	0.212%
24	10.634	1447	1452	1460	rBV	410540	510328	31.66%	3.679%
25	10.710	1460	1465	1479	rBV	740603	973951	60.43%	7.021%
26	10.945	1498	1505	1510	rBV	62453	79899	4.96%	0.576%
27	11.063	1517	1525	1531	rBV3	14515	22738	1.41%	0.164%
28	11.316	1564	1568	1573	rVB4	13671	19613	1.22%	0.141%
29	11.410	1579	1584	1592	rVB	607941	753784	46.77%	5.434%
30	11.651	1619	1625	1630	rBV6	7656	19709	1.22%	0.142%
31	11.857	1656	1660	1667	rBV4	11334	18273	1.13%	0.132%
32	11.933	1668	1673	1686	rBV	197769	310590	19.27%	2.239%
33	12.433	1754	1758	1765	rVB	19930	30734	1.91%	0.222%
34	12.628	1785	1791	1802	rBV3	97073	243969	15.14%	1.759%
35	12.716	1802	1806	1819	rVB	42356	79975	4.96%	0.577%
36	12.992	1848	1853	1861	rVB	874120	1094901	67.94%	7.893%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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	13.569	1947	1951	1960	rVB2	10268	17425	1.08%	0.126%
38	13.898	2002	2007	2022	rBV	39002	95108	5.90%	0.686%
39	14.045	2027	2032	2041	rVB	349760	470539	29.20%	3.392%
40	14.216	2058	2061	2075	rVB5	8573	23722	1.47%	0.171%
41	14.674	2135	2139	2144	rBV2	19115	26725	1.66%	0.193%
42	14.904	2174	2178	2184	rVB	60780	80873	5.02%	0.583%
43	15.169	2220	2223	2231	rVB2	12933	19657	1.22%	0.142%
44	15.527	2277	2284	2294	rBV	342416	566948	35.18%	4.087%
45	15.674	2305	2309	2318	rVB6	12350	20531	1.27%	0.148%
46	16.004	2361	2365	2370	rBV	13226	20192	1.25%	0.146%
47	18.245	2741	2746	2756	rVB2	16920	44546	2.76%	0.321%

Sum of corrected areas: 13872353

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
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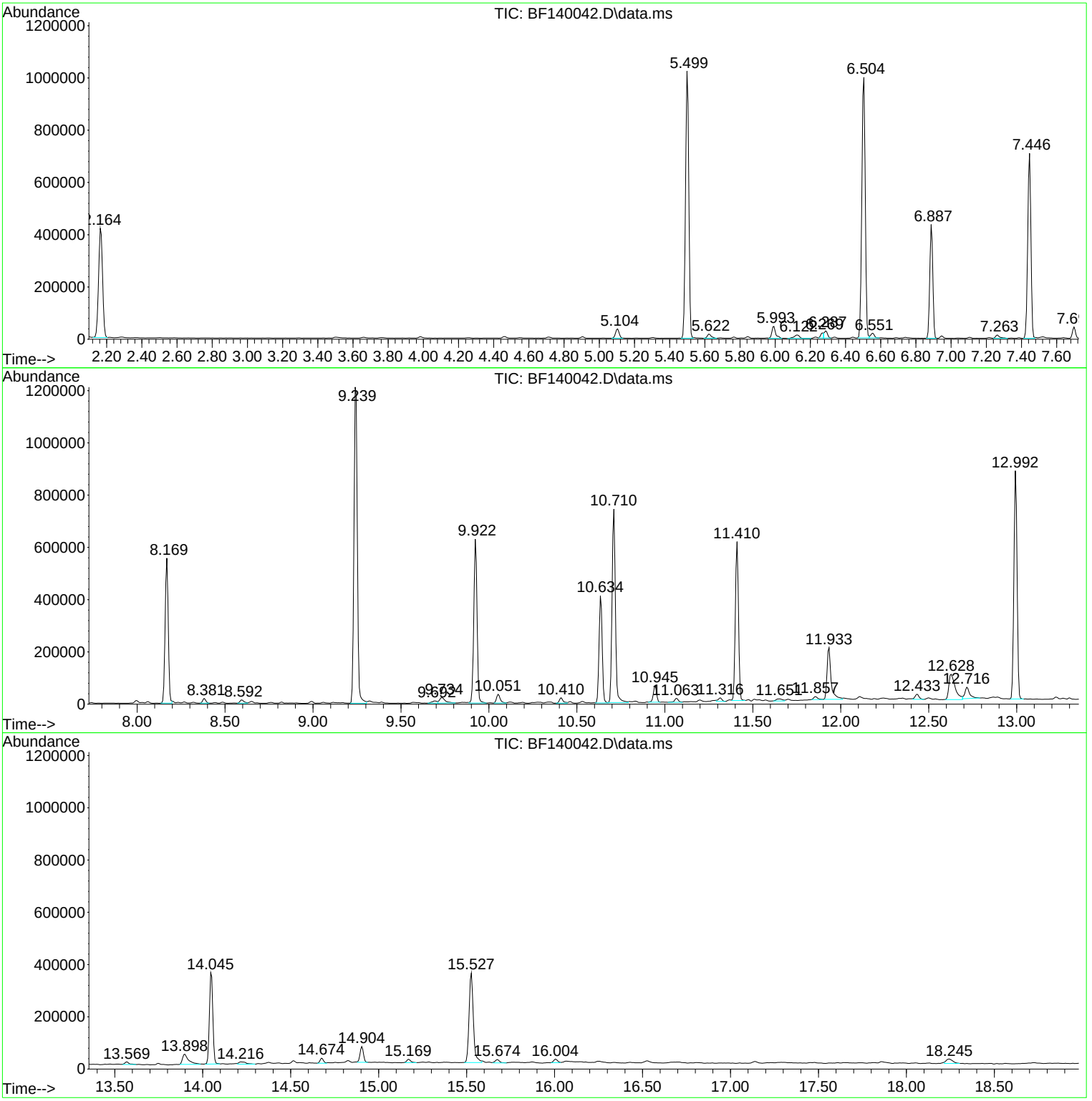
Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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

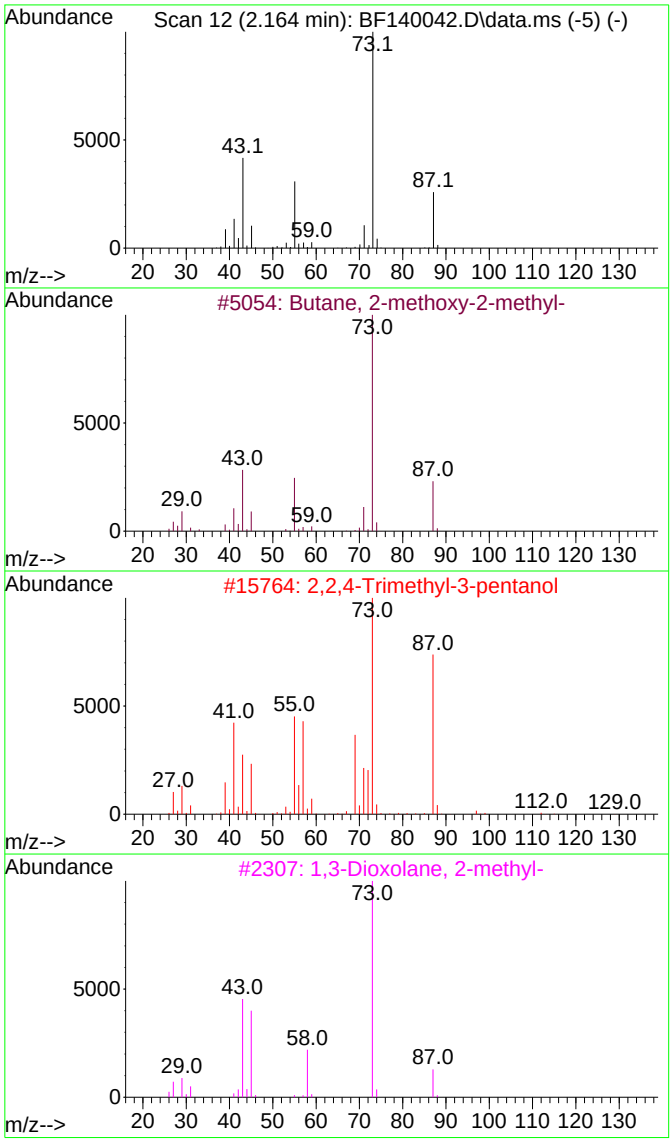
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

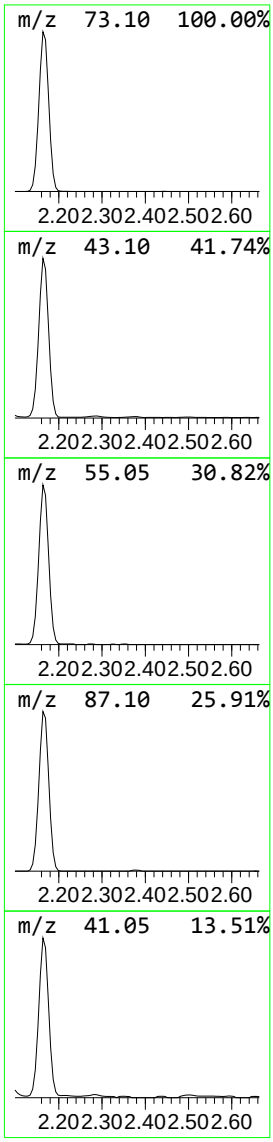
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.164	25.06 ng	656746	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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

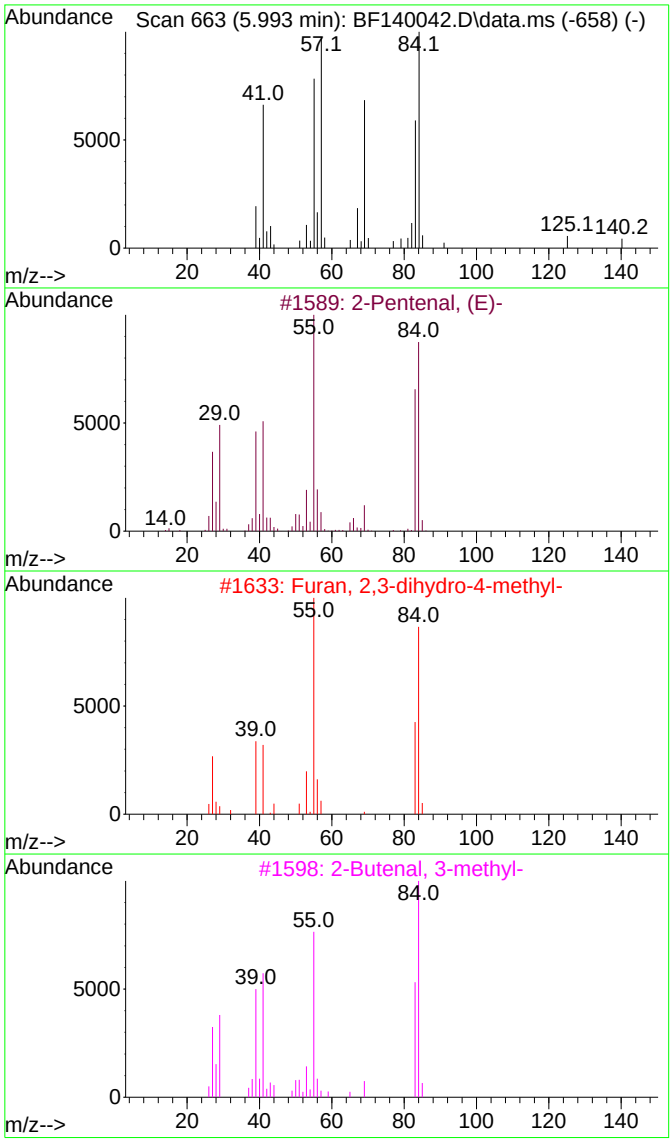
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

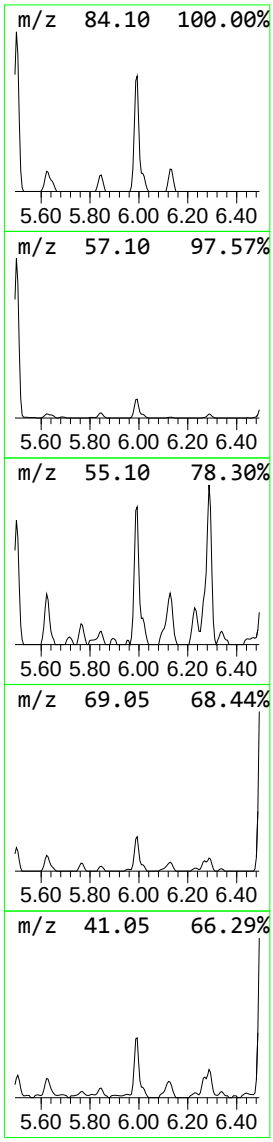
****

Peak Number 2 2-Pentenal, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.993	2.60 ng	68085	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentenal, (E)-	84	C5H8O	001576-87-0	59
2	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	53
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	53
4	1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	50
5	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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

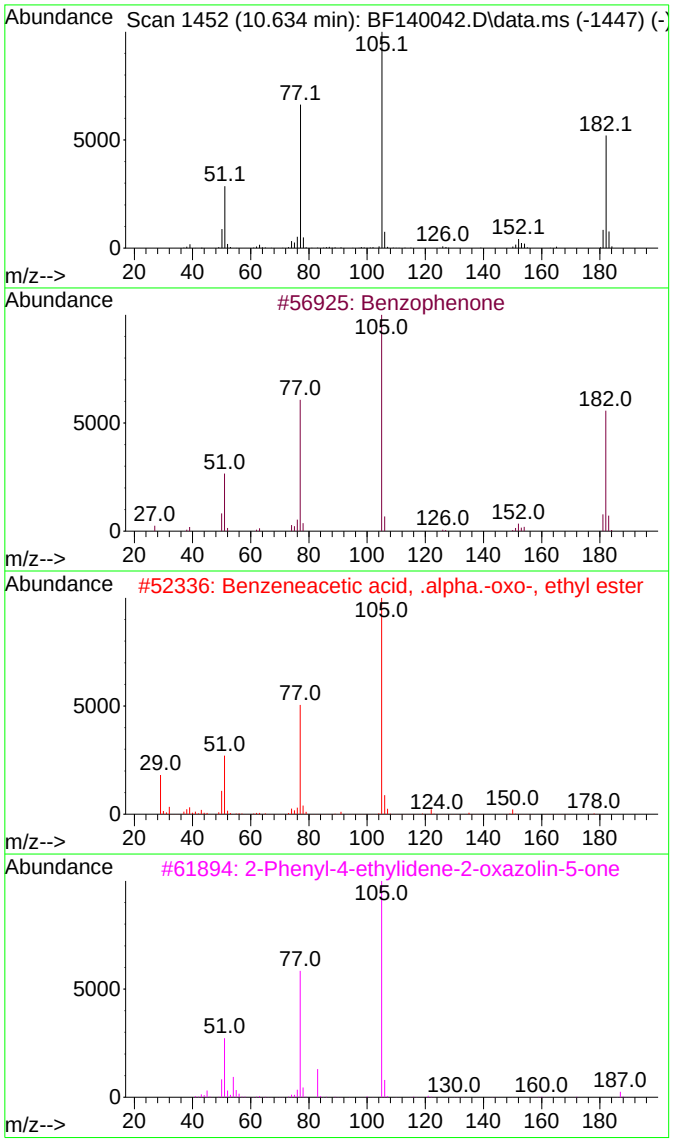
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

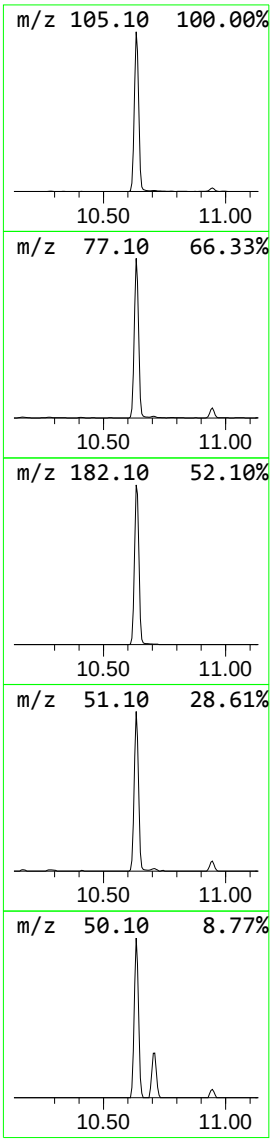
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	12.70 ng	510328	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	47
3	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

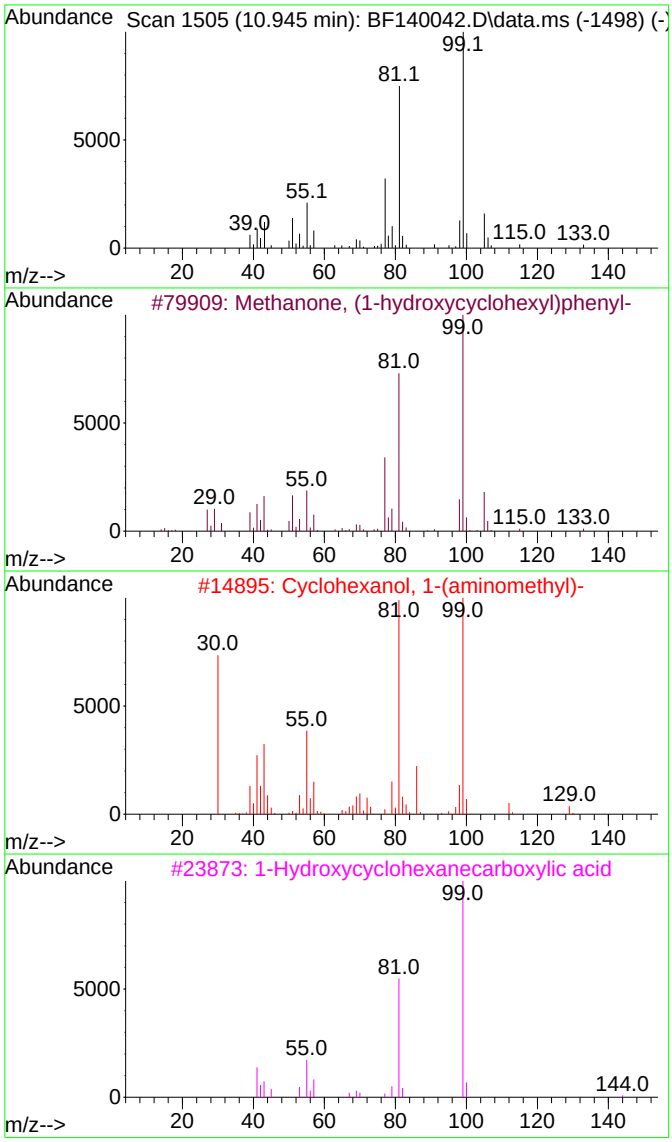
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

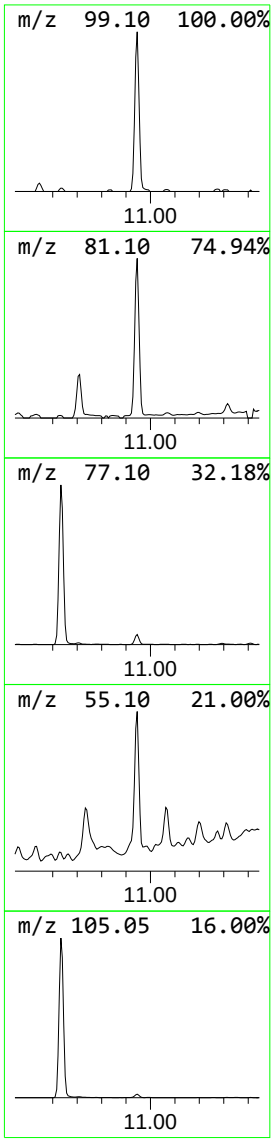
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	2.12 ng	79899	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	64
3	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	45
4	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	45
5	2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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

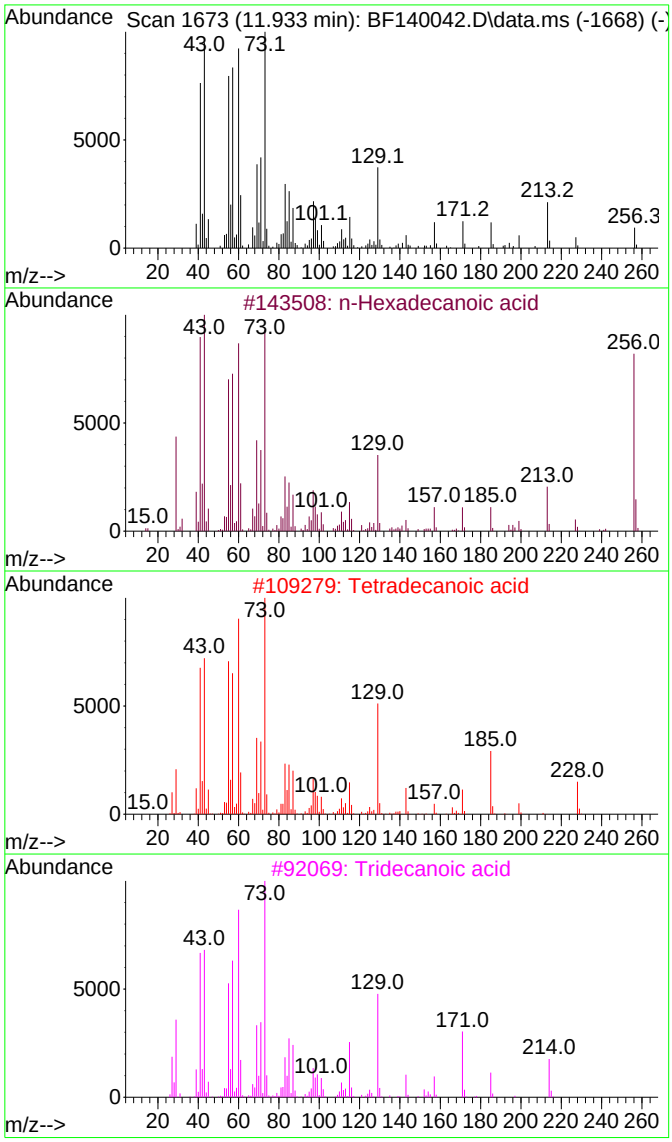
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

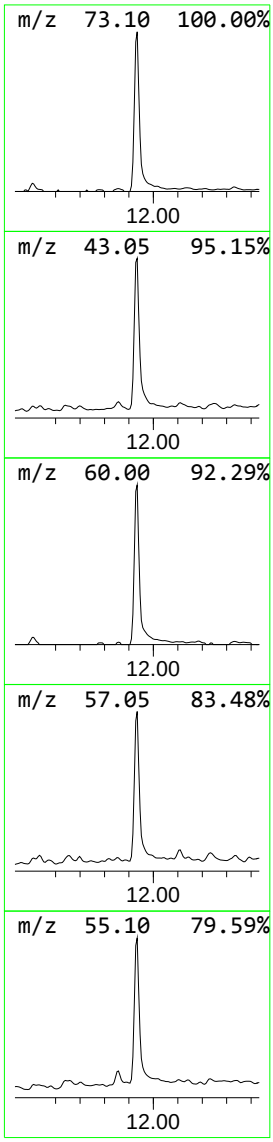
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.934	8.24 ng	310590	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	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
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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

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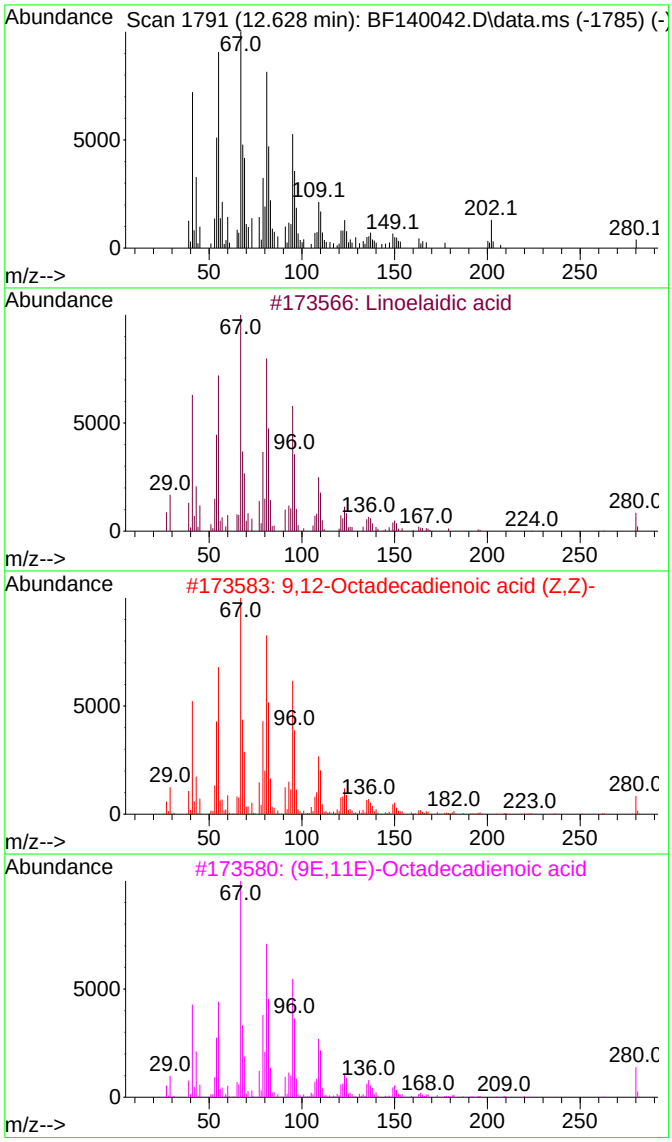
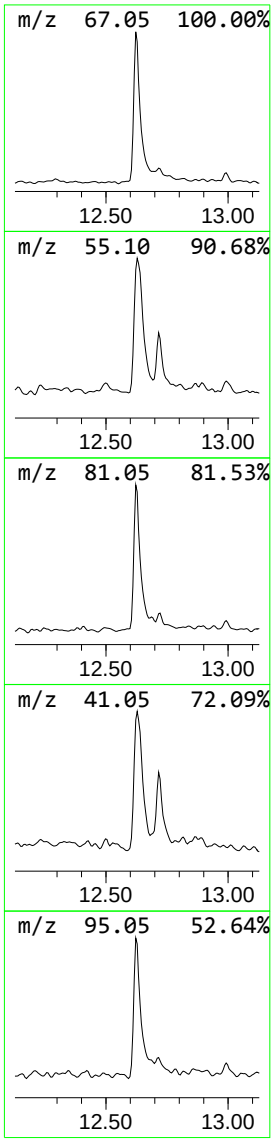
Peak Number 6 Linoelaidic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.628	6.47 ng	243969	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	98
3	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	98
4	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
5	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94





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Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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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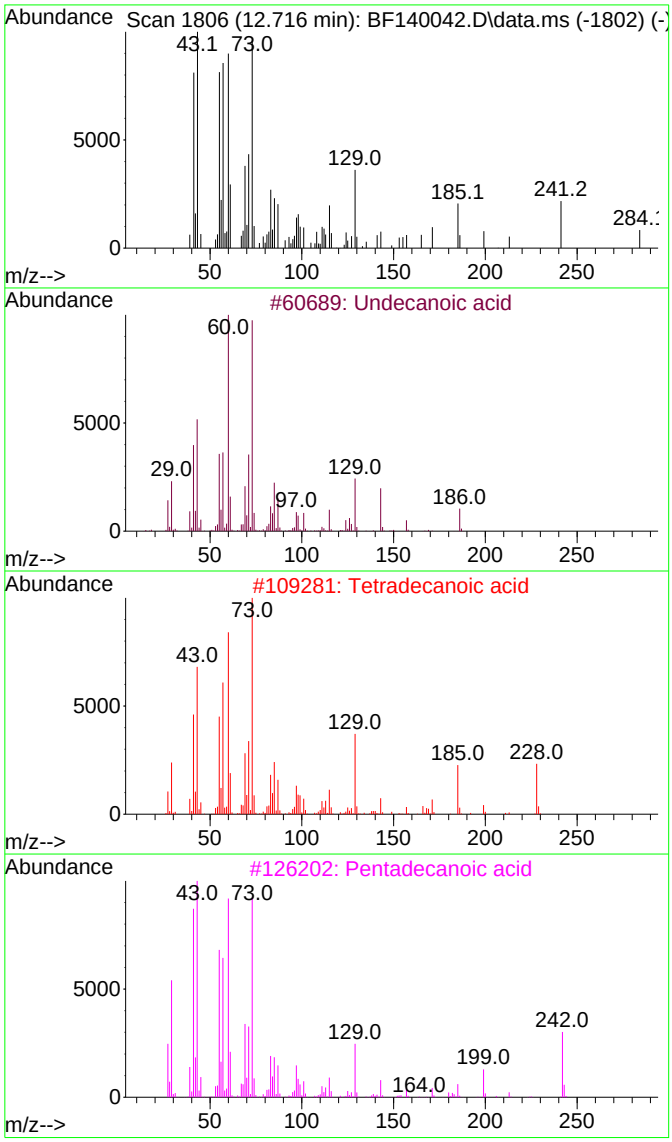
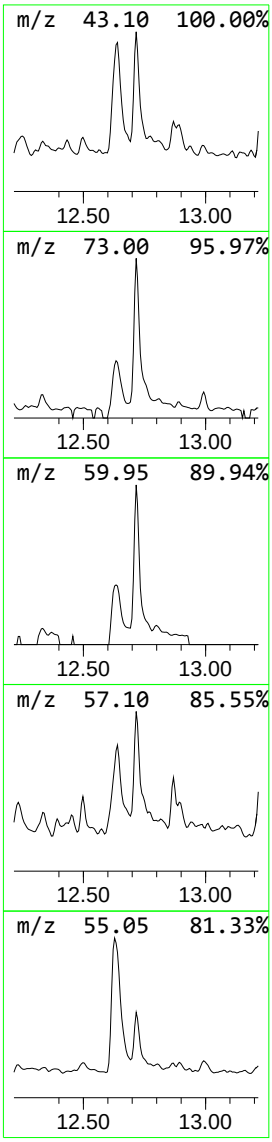
Peak Number 7 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.12 ng	79975	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	90
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D20241001-01-04

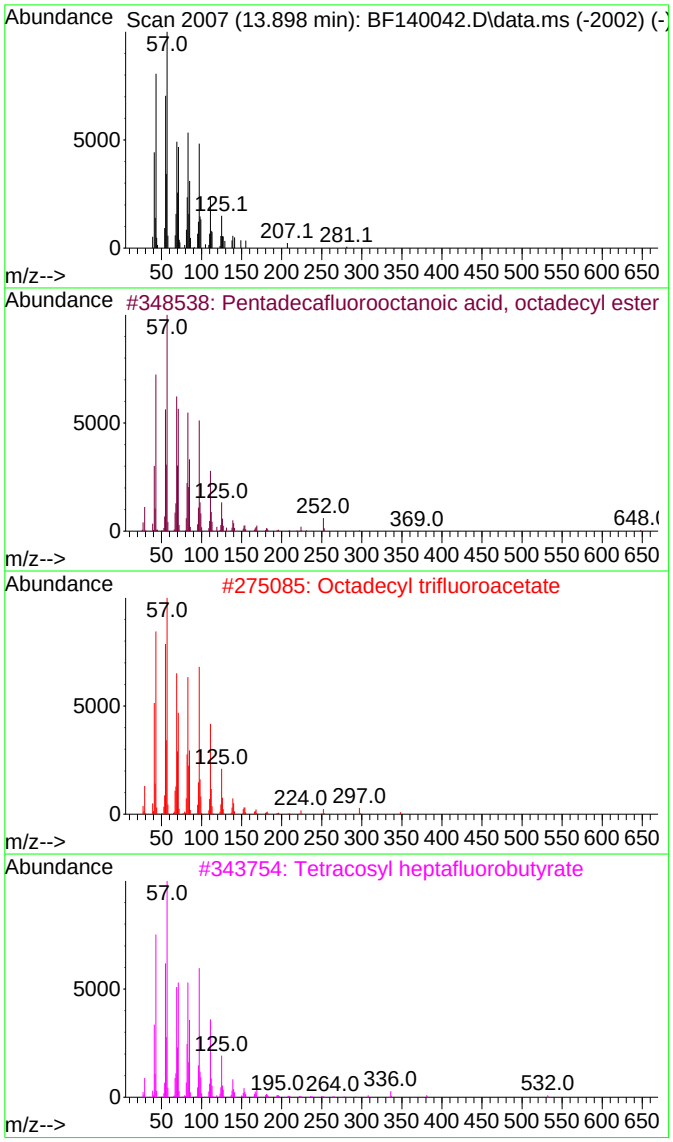
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

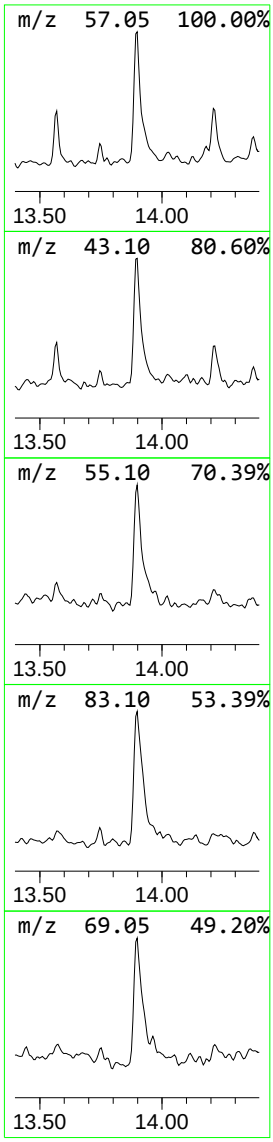
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.04 ng	95108	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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

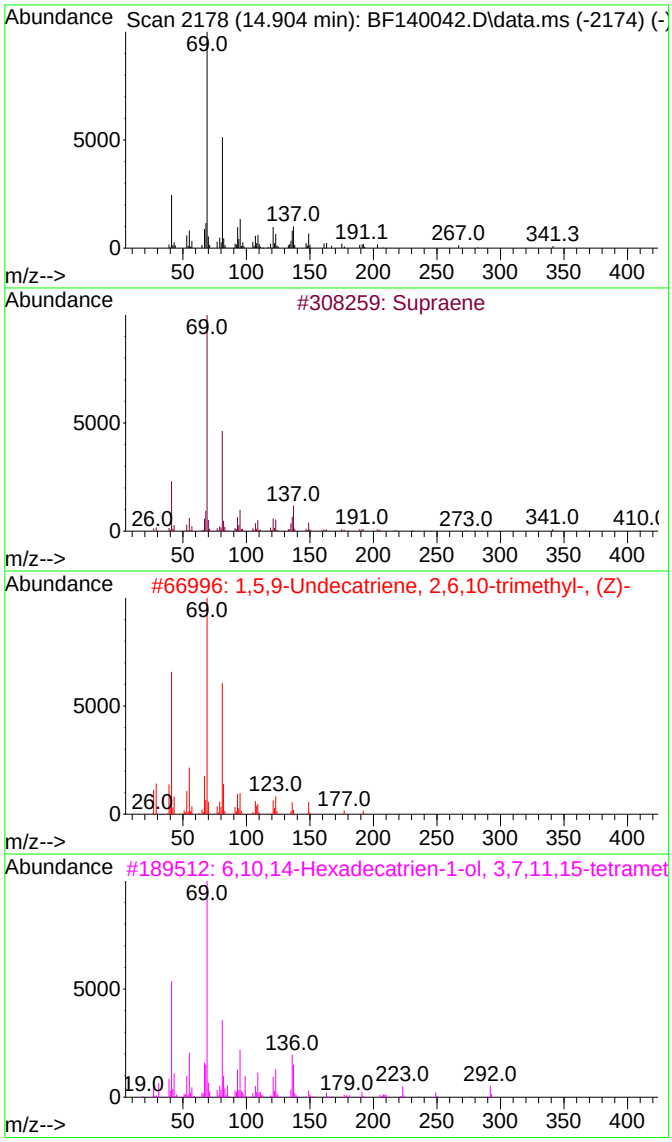
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

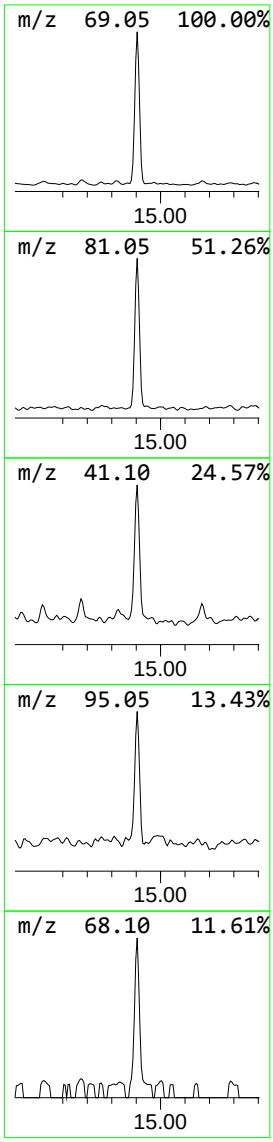
****

Peak Number 9 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	2.85 ng	80873	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	78
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	74
5	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102524\
Data File : BF140042.D
Acq On : 25 Oct 2024 17:25
Operator : RC/JU
Sample : P4485-01
Misc :
ALS Vial : 18 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...	2.164	25.1	ng	656746	1	6.887	524205	20.0
2-Pentenal, (E)-	5.993	2.6	ng	68085	1	6.887	524205	20.0
Benzophenone	10.634	12.7	ng	510328	3	9.922	803468	20.0
Methanone, (1-h...	10.945	2.1	ng	79899	4	11.410	753784	20.0
n-Hexadecanoic ...	11.934	8.2	ng	310590	4	11.410	753784	20.0
Linoelaidic acid	12.628	6.5	ng	243969	4	11.410	753784	20.0
Undecanoic acid	12.716	2.1	ng	79975	4	11.410	753784	20.0
Pentadecafluoro...	13.898	4.0	ng	95108	5	14.045	470539	20.0
Supraene	14.904	2.9	ng	80873	6	15.527	566948	20.0