LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123124\
Data File : BF141053.D
Acq On : 31 Dec 2024 12:42
Operator : RC/JU
Sample : P5398-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 341-349

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-BF122624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141053.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	12	17	39	rVB2	105732	204926	3.46%	0.458%
2	5.046	497	502	511	rVB	51335	86953	1.47%	0.194%
3	5.393	556	561	563	rBV	164916	194250	3.28%	0.434%
4	5.440	563	569	575	rVB	3599400	5246981	88.58%	11.722%
5	6.393	720	731	734	rBV2	35044	64329	1.09%	0.144%
6	6.445	734	740	746	rBV	3694613	5203369	87.84%	11.624%
7	6.828	794	805	810	rVB	1161782	1427841	24.10%	3.190%
8	7.387	891	900	905	rBV	2647776	3422685	57.78%	7.646%
9	7.639	939	943	953	rVB	126427	158851	2.68%	0.355%
10	8.110	1017	1023	1031	rBV	1427431	1867946	31.53%	4.173%
11	8.322	1052	1059	1066	rVB	69302	98200	1.66%	0.219%
12	9.181	1199	1205	1210	rBV	4733916	5923602	100.00%	13.233%
13	9.722	1293	1297	1301	rBV	39631	64586	1.09%	0.144%
14	9.857	1315	1320	1325	rBV	1563531	1952790	32.97%	4.363%
15	10.269	1386	1390	1394	rBV3	54324	67847	1.15%	0.152%
16	10.569	1437	1441	1448	rBV	936685	1211646	20.45%	2.707%
17	10.645	1449	1454	1465	rVV	2464268	3232137	54.56%	7.221%
18	10.880	1490	1494	1498	rBV	150562	183644	3.10%	0.410%
19	11.345	1568	1573	1580	rBV	1187230	1653936	27.92%	3.695%
20	11.575	1608	1612	1620	rBV2	158710	320876	5.42%	0.717%
21	11.875	1659	1663	1673	rBV	722508	1006745	17.00%	2.249%
22	12.398	1749	1752	1756	rBV	85622	103585	1.75%	0.231%
23	12.557	1774	1779	1783	rBV	342252	478075	8.07%	1.068%
24	12.663	1793	1797	1810	rVB3	211860	380539	6.42%	0.850%
25	12.780	1813	1817	1821	rBV	331822	436584	7.37%	0.975%
26	12.933	1837	1843	1850	rVB	3042725	3995445	67.45%	8.926%
27	13.839	1993	1997	2013	rVB4	204651	417110	7.04%	0.932%
28	13.980	2016	2021	2032	rVB2	1163351	2008696	33.91%	4.487%
29	14.851	2166	2169	2175	rVB2	123701	173733	2.93%	0.388%
30	15.021	2194	2198	2208	rBV	364237	829991	14.01%	1.854%
31	15.227	2230	2233	2238	rVB	155877	219934	3.71%	0.491%
32	15.321	2246	2249	2255	rVB	209352	300788	5.08%	0.672%
33	15.380	2255	2259	2264	rBV	279764	415420	7.01%	0.928%
34	15.445	2265	2270	2283	rVB2	758747	1408256	23.77%	3.146%

Sum of corrected areas: 44762296

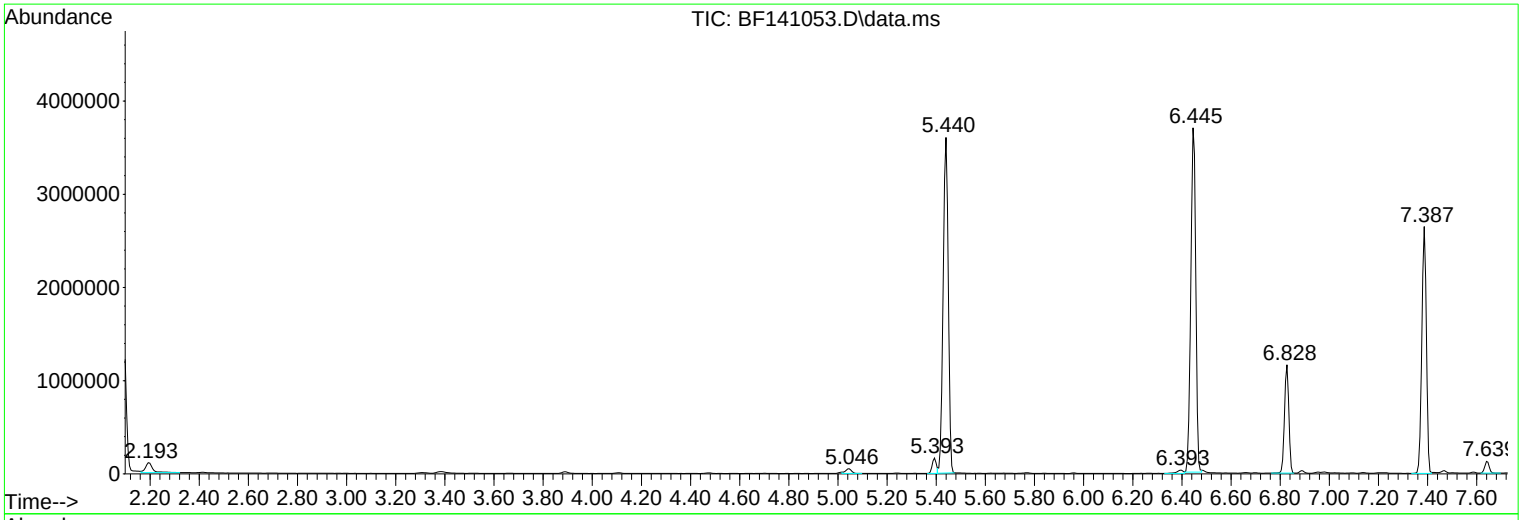
Instrument :
BNA_F
ClientSampleId :
341-349

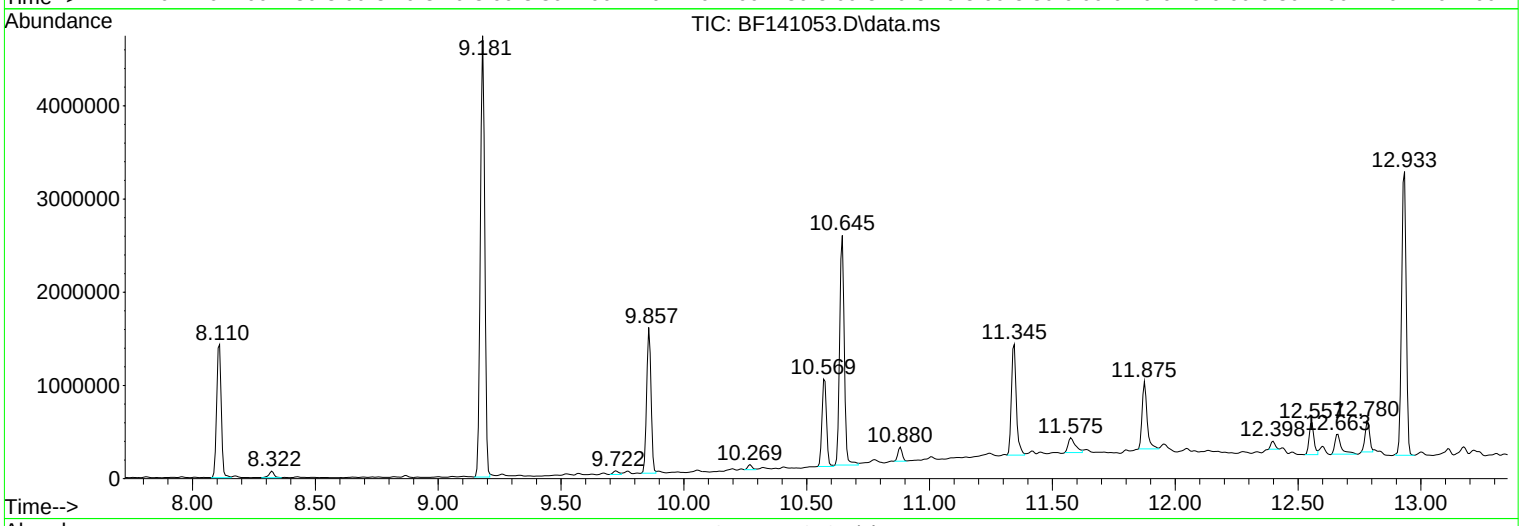
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123124\
Data File : BF141053.D
Acq On : 31 Dec 2024 12:42
Operator : RC/JU
Sample : P5398-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

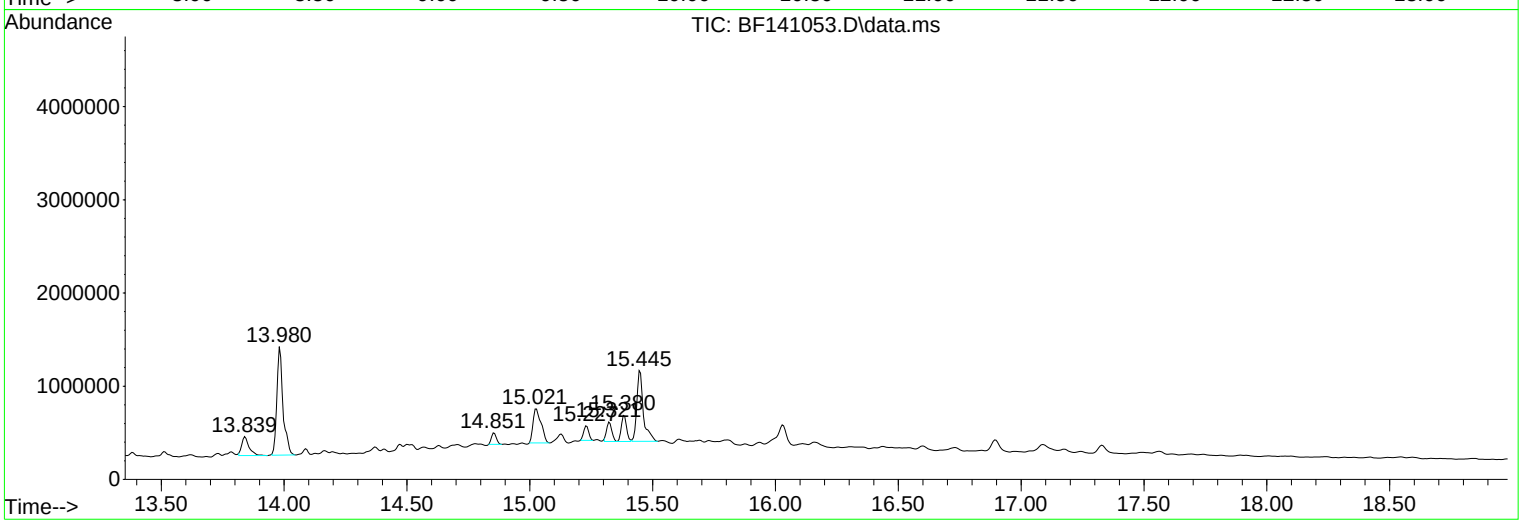
Instrument :
BNA_F
ClientSampleId :
341-349

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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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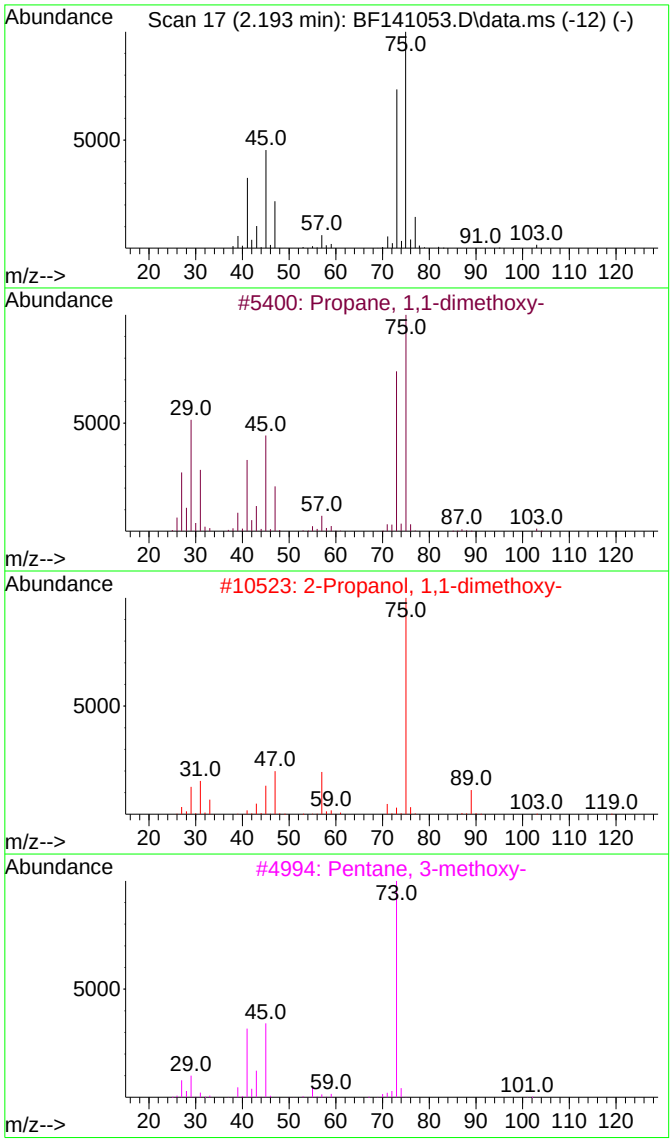
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

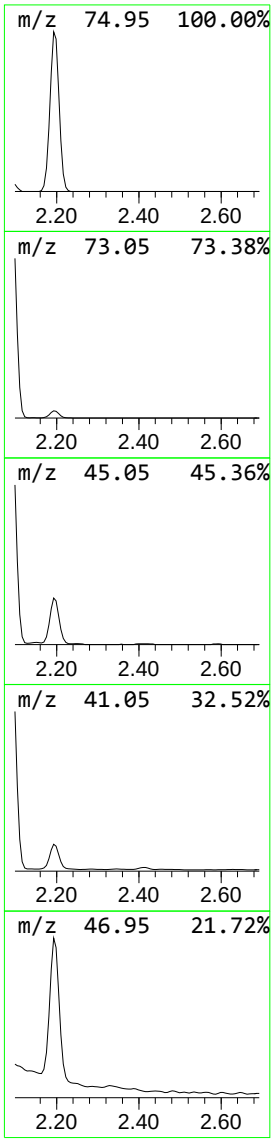
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	2.87 ng	204926	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	9
5	Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
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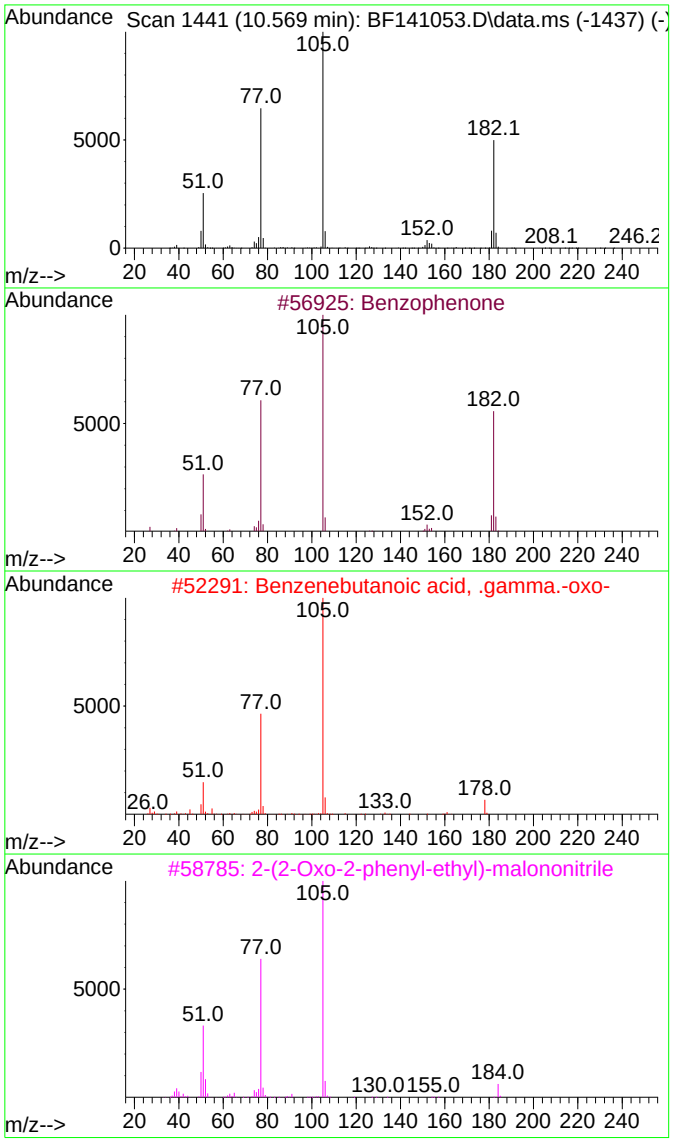
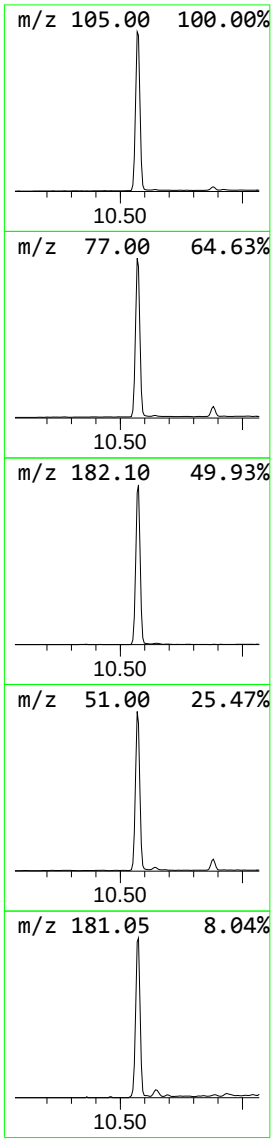
****

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.569	12.41 ng	1211650	Acenaphthene-d10	9.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





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Operator : RC/JU
Sample : P5398-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
341-349

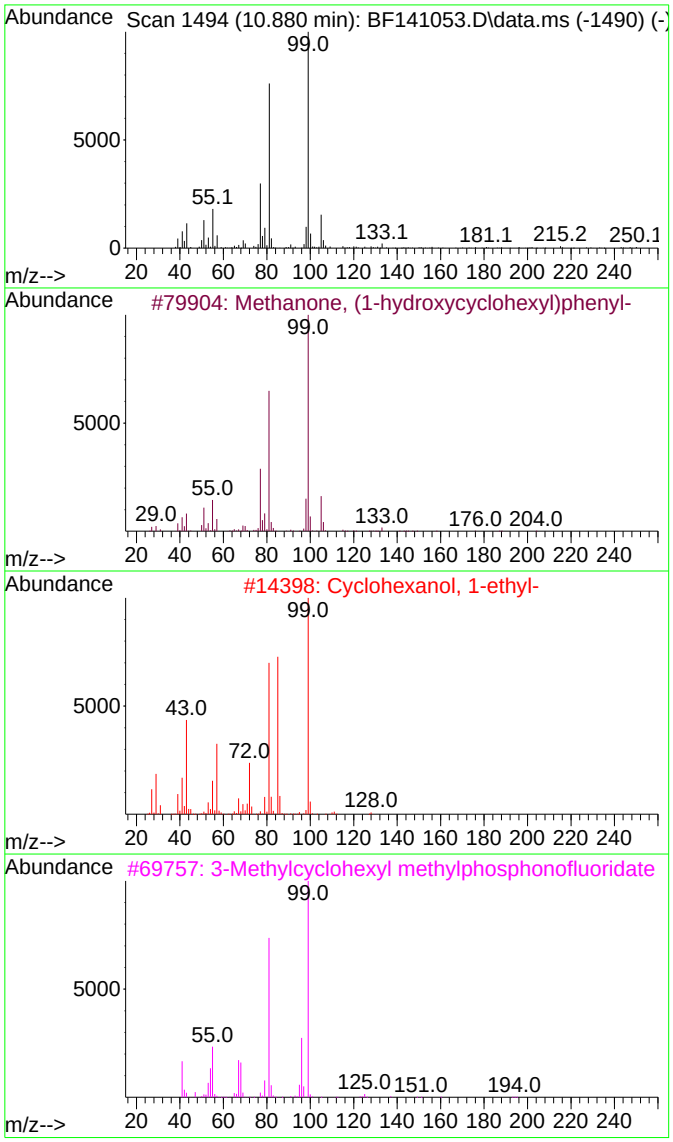
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

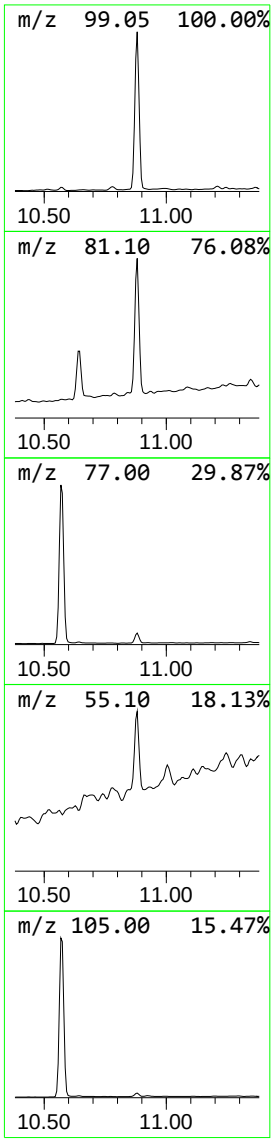
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methanone, (1-hydroxycycloh... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.881	2.22 ng	183644	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	59
3	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	45
4	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	45
5	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	38





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Sample : P5398-01
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
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TIC Library : C:\Database\NIST20.L
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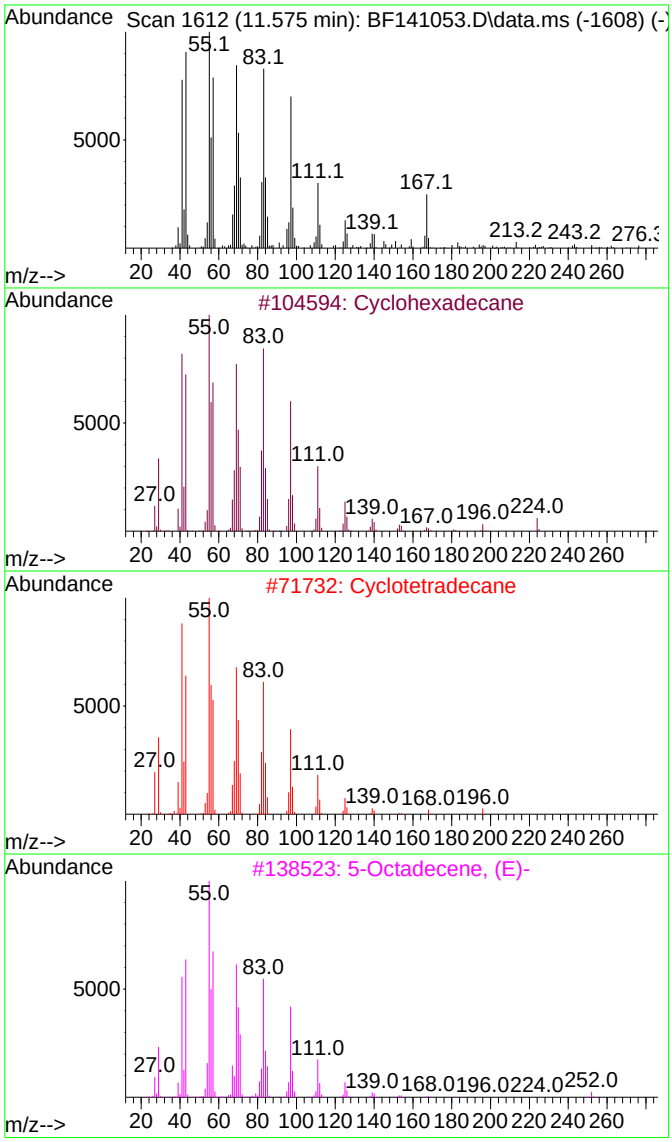
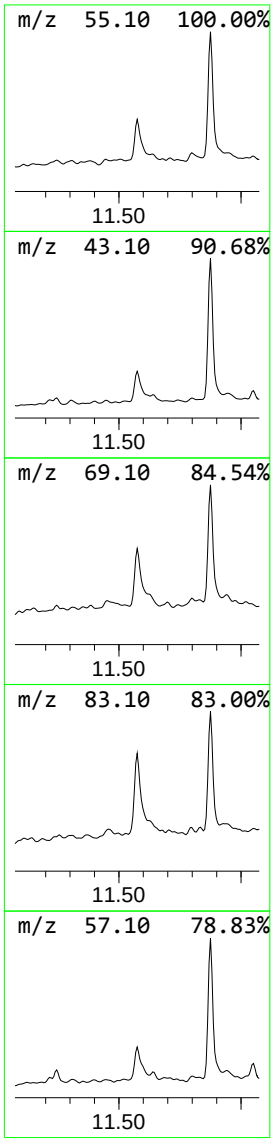
****

Peak Number 4 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.575	3.88 ng	320876	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	98
2	Cyclotetradecane	196	C14H28	000295-17-0	97
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
4	Cyclododecane	168	C12H24	000294-62-2	94
5	Acetic acid, trifluoro-, dodecyl...	282	C14H25F3O2	006222-00-0	94





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Sample : P5398-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
341-349

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

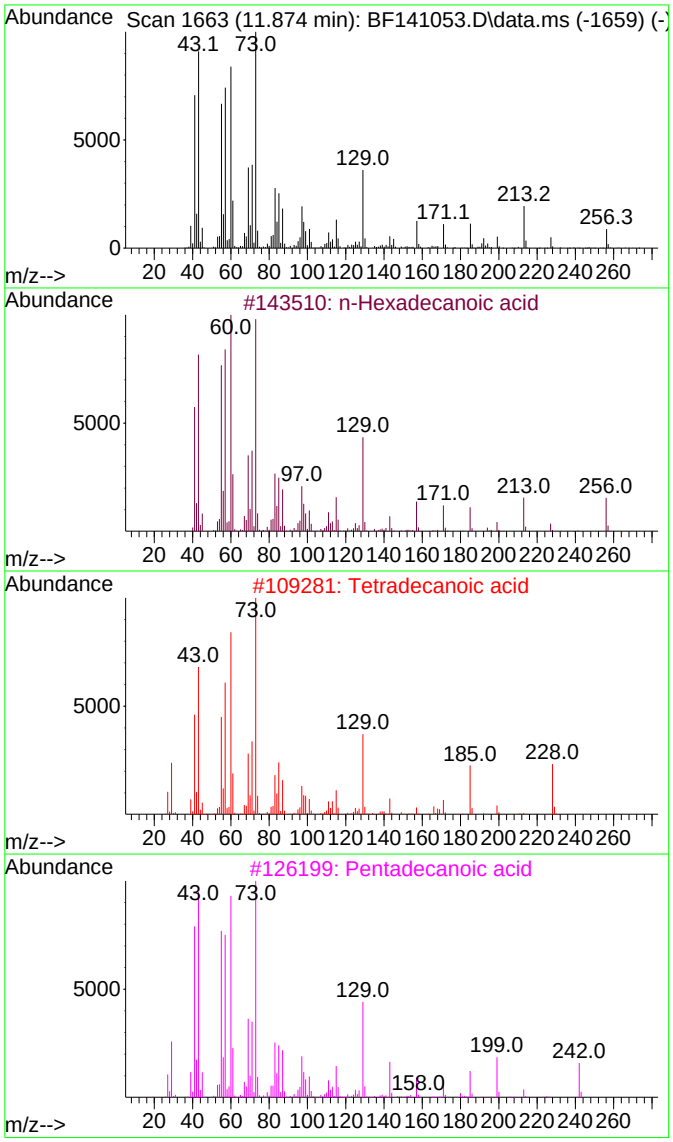
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

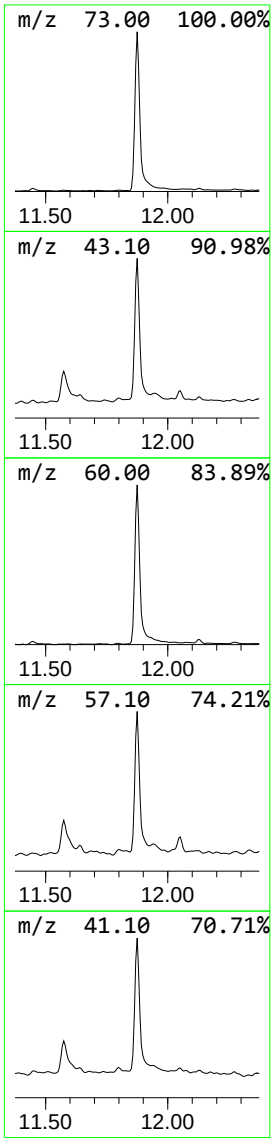
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	12.17 ng	1006750	Phenanthrene-d10	11.345

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





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Sample : P5398-01
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Instrument :
BNA_F
ClientSampleId :
341-349

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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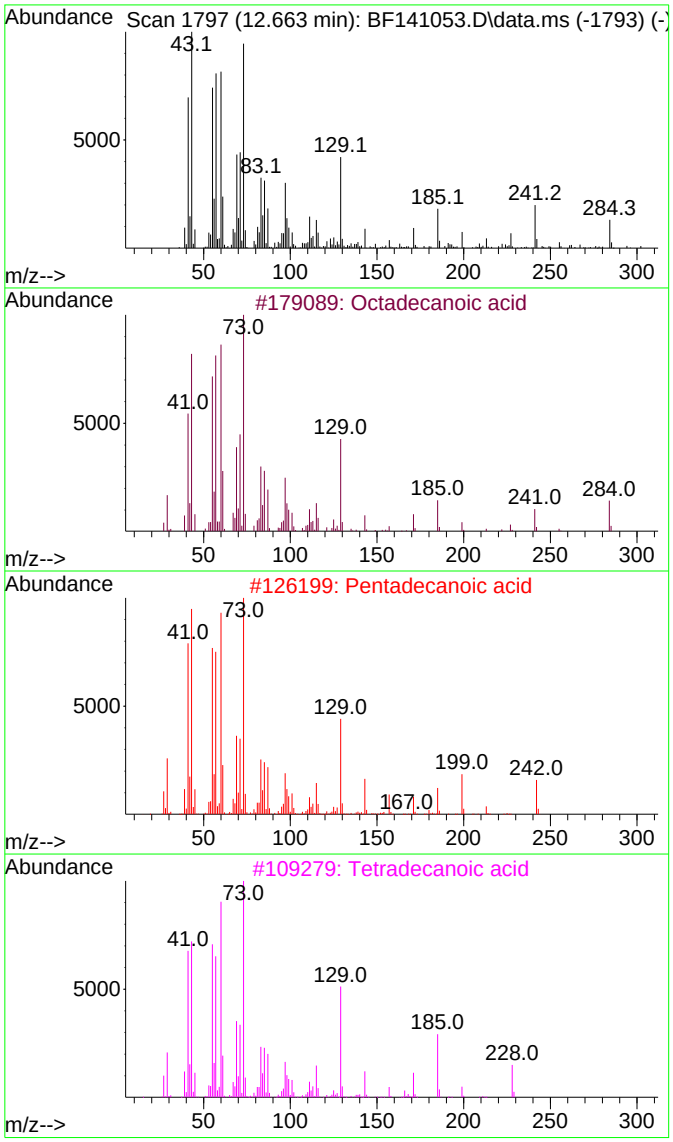
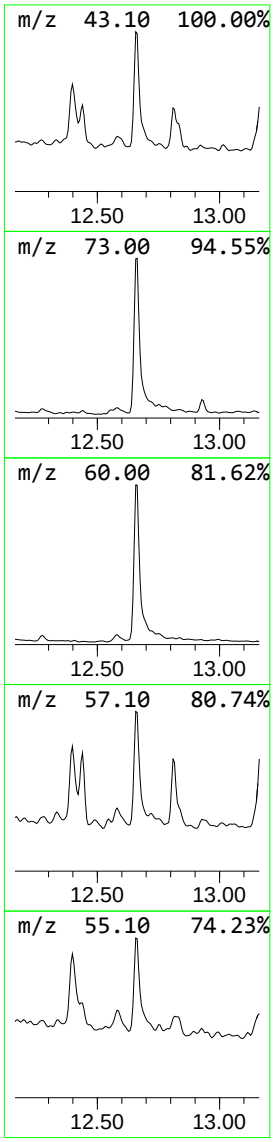
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	4.60 ng	380539	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	50





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Sample : P5398-01
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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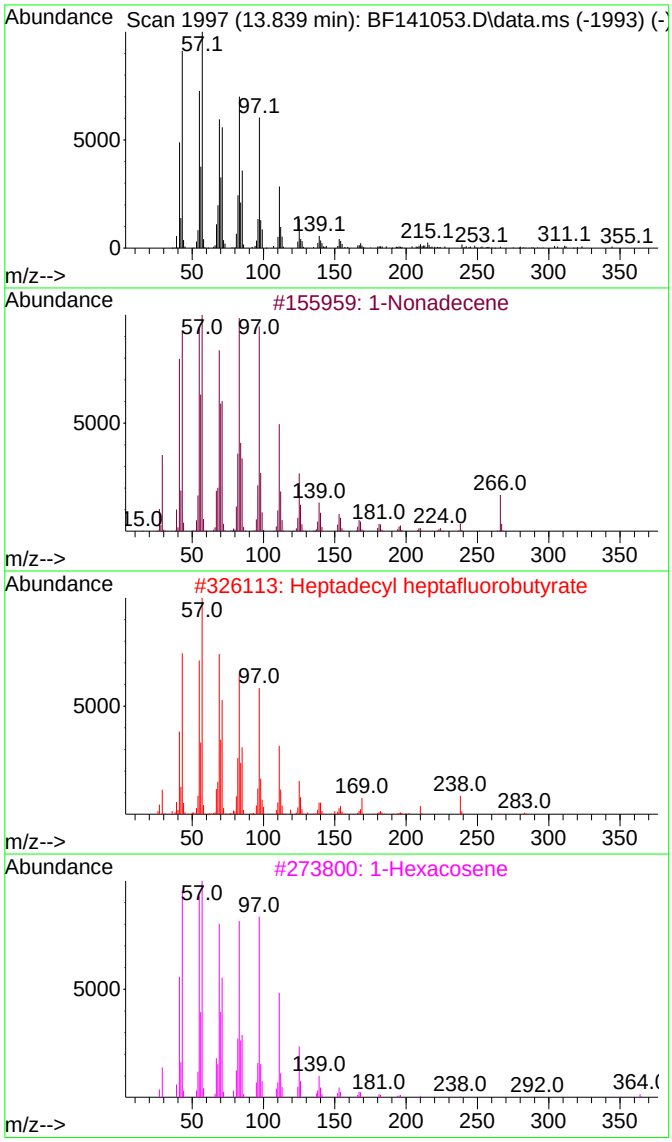
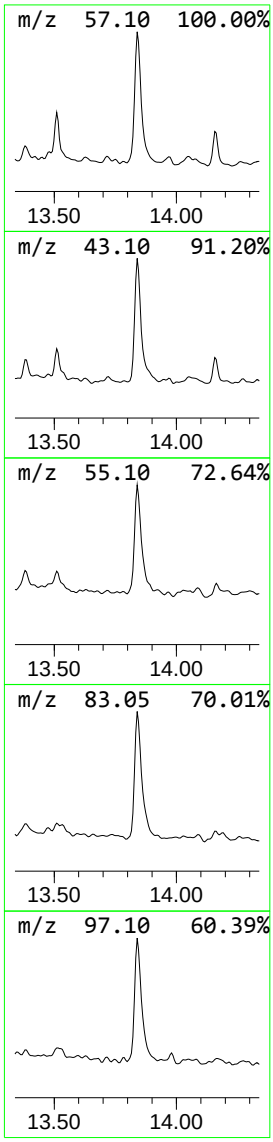
****

Peak Number 7 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	4.15 ng	417110	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	97
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Hexacosene	364	C26H52	018835-33-1	94
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





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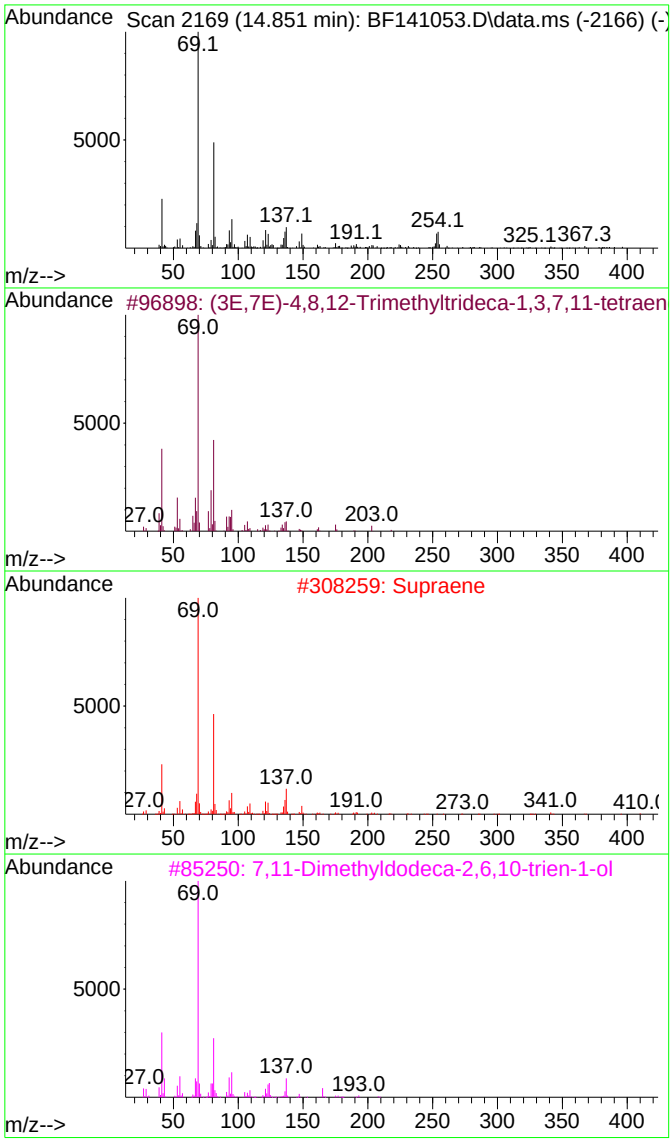
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

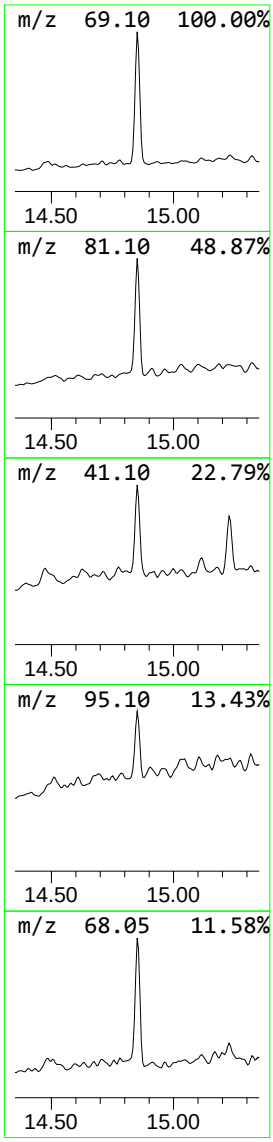
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (3E,7E)-4,8,12-Trimethyltri... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	2.47 ng	173733	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	72
2	Supraene	410	C30H50	007683-64-9	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	59





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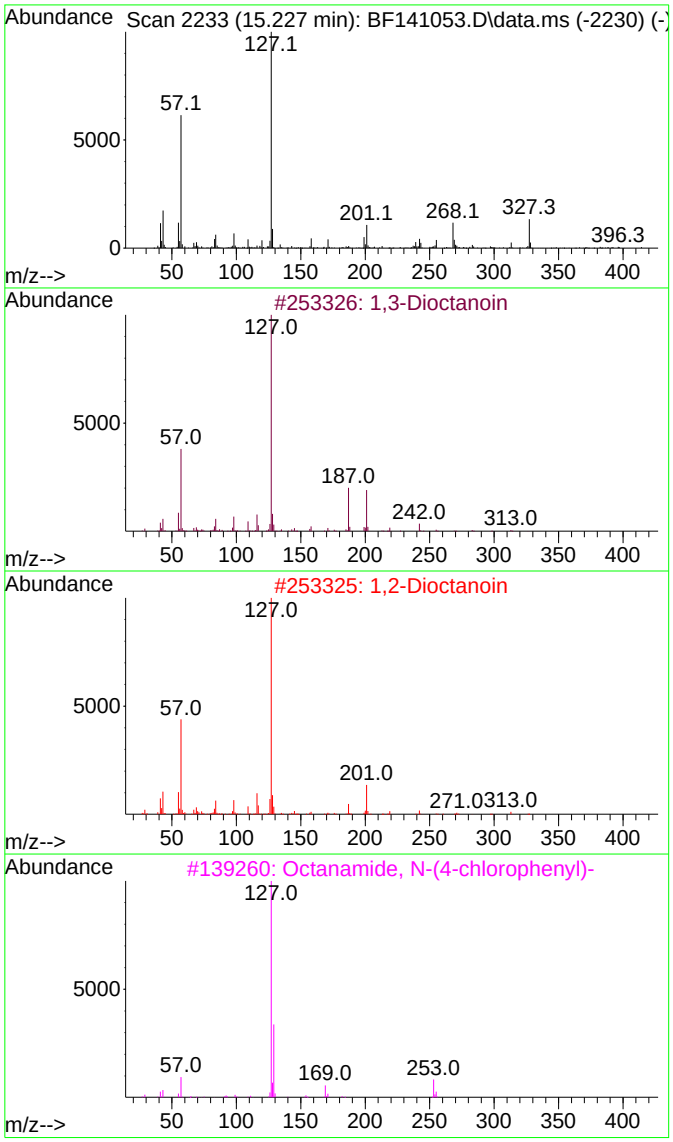
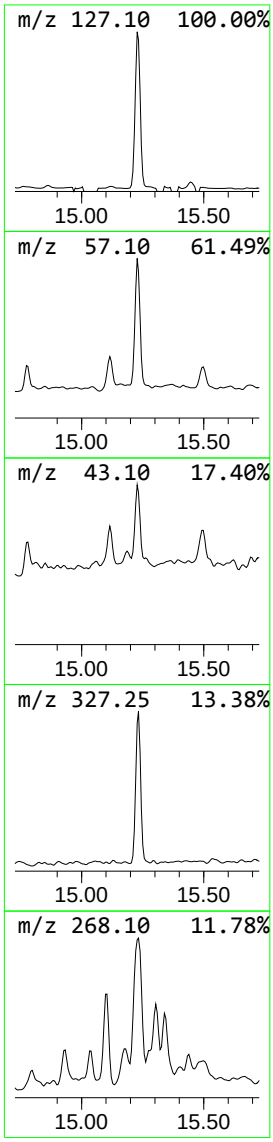
Peak Number 9 1,3-Dioctanoin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	3.12 ng	219934	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioctanoin	344	C19H36O5	001429-66-9	53
2	1,2-Dioctanoin	344	C19H36O5	001069-87-0	53
3	Octanamide, N-(4-chlorophenyl)-	253	C14H20ClNO	1000340-16-6	50
4	3-Fluoro-5-methoxypyridine	127	C6H6FNO	1060801-62-8	49
5	Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123124\
Data File : BF141053.D
Acq On : 31 Dec 2024 12:42
Operator : RC/JU
Sample : P5398-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
341-349

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

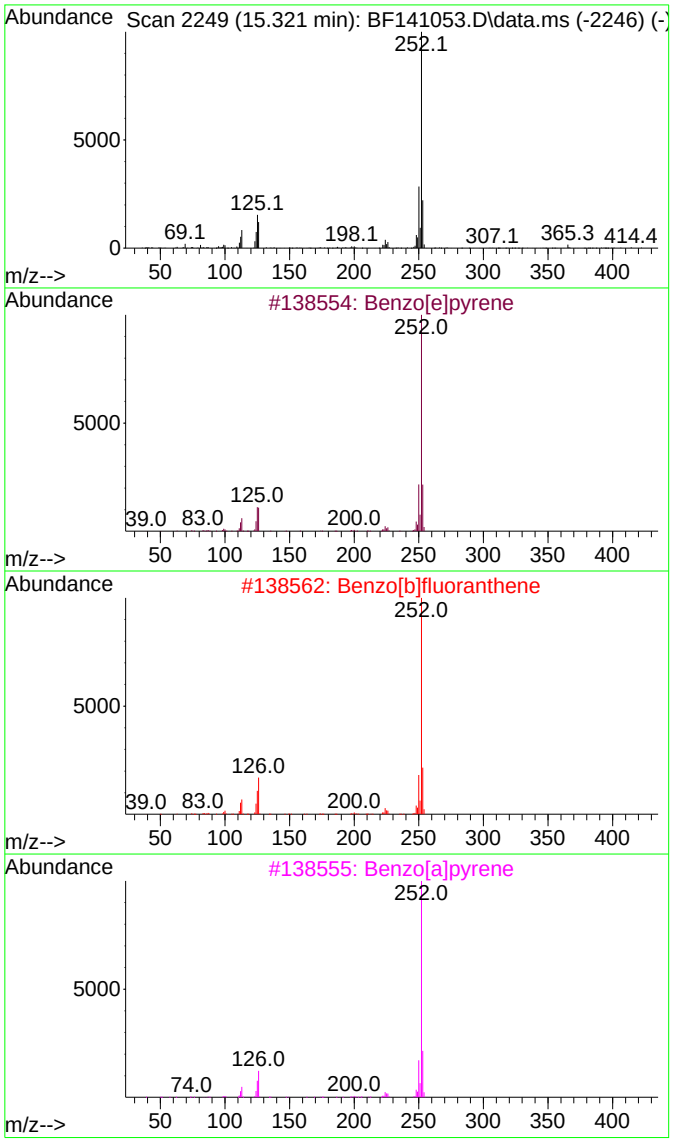
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

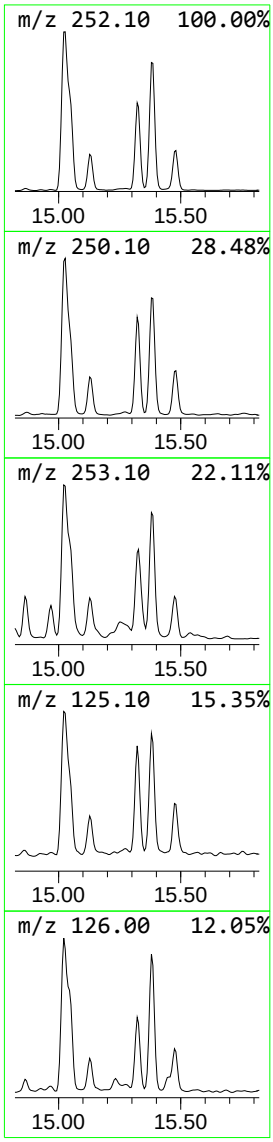
****

Peak Number 10 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	4.27 ng	300788	Perylene-d12	15.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123124\
Data File : BF141053.D
Acq On : 31 Dec 2024 12:42
Operator : RC/JU
Sample : P5398-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
341-349

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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
Propane, 1,1-di...	2.193	2.9	ng	204926	1	6.828	1427840	20.0
Benzophenone	10.569	12.4	ng	1211650	3	9.857	1952790	20.0
Methanone, (1-h...	10.881	2.2	ng	183644	4	11.345	1653940	20.0
Cyclohexadecane	11.575	3.9	ng	320876	4	11.345	1653940	20.0
n-Hexadecanoic ...	11.874	12.2	ng	1006750	4	11.345	1653940	20.0
Octadecanoic acid	12.663	4.6	ng	380539	4	11.345	1653940	20.0
1-Nonadecene	13.839	4.2	ng	417110	5	13.980	2008700	20.0
(3E,7E)-4,8,12-...	14.851	2.5	ng	173733	6	15.445	1408260	20.0
1,3-Dioctanoin	15.227	3.1	ng	219934	6	15.445	1408260	20.0
Benzo[e]pyrene	15.321	4.3	ng	300788	6	15.445	1408260	20.0