LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051520\
Data File : BF120329.D
Acq On : 15 May 2020 18:47
Operator : MA/SJ
Sample : L2646-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-B-S

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-BF051420.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.092	338	341	359	rBV	91231	192661	4.65%	0.436%
2	4.775	455	457	467	rBV	82208	110382	2.66%	0.250%
3	5.222	530	533	552	rBV	2721823	3336781	80.54%	7.546%
4	5.557	587	590	597	rBV	33731	61883	1.49%	0.140%
5	6.263	707	710	741	rBV	2704741	3400086	82.07%	7.689%
6	6.616	766	770	780	rBV	1249305	1631829	39.39%	3.690%
7	6.769	791	796	822	rVB	2431022	2852477	68.85%	6.451%
8	7.181	862	866	897	rBV	1835920	2278659	55.00%	5.153%
9	7.386	898	901	906	rVB	52715	52195	1.26%	0.118%
10	7.898	984	988	1012	rBV	2015770	2280085	55.03%	5.156%
11	8.975	1166	1171	1183	rBV	4201400	4143075	100.00%	9.369%
12	9.374	1235	1239	1249	rVB	538427	543938	13.13%	1.230%
13	9.645	1280	1285	1311	rBV	2487520	2572248	62.09%	5.817%
14	10.439	1415	1420	1438	rBV	2163428	2496766	60.26%	5.646%
15	10.816	1481	1484	1489	rBV	96509	122095	2.95%	0.276%
16	11.133	1533	1538	1549	rBV	2401352	2800184	67.59%	6.332%
17	11.257	1556	1559	1566	rVB2	63311	78410	1.89%	0.177%
18	11.445	1586	1591	1600	rBV9	17440	48956	1.18%	0.111%
19	11.527	1602	1605	1613	rVB4	34262	56937	1.37%	0.129%
20	11.598	1614	1617	1626	rBV2	262241	405733	9.79%	0.918%
21	11.680	1626	1631	1639	rBV	1092767	1303519	31.46%	2.948%
22	11.739	1639	1641	1644	rVB	45162	45470	1.10%	0.103%
23	11.921	1670	1672	1677	rVB2	65435	63647	1.54%	0.144%
24	12.339	1739	1743	1746	rBV	283865	286725	6.92%	0.648%
25	12.380	1746	1750	1761	rVV	177324	367066	8.86%	0.830%
26	12.457	1761	1763	1775	rVB2	202528	316440	7.64%	0.716%
27	12.568	1776	1782	1785	rBV	225963	256938	6.20%	0.581%
28	12.715	1803	1807	1817	rBV	3798983	3771040	91.02%	8.528%
29	12.898	1832	1838	1842	rVB2	33812	53496	1.29%	0.121%
30	12.963	1842	1849	1853	rVV5	29873	45445	1.10%	0.103%
31	13.004	1853	1856	1862	rVB2	32835	45270	1.09%	0.102%
32	13.627	1958	1962	1968	rBV2	205439	305350	7.37%	0.691%
33	13.768	1978	1986	1998	rBV	1856031	2275599	54.93%	5.146%
34	13.945	2009	2016	2019	rBV2	74366	98006	2.37%	0.222%

LSC Area Percent Report

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Operator : MA/SJ
Sample : L2646-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-B-S

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-BF051420.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.251	2063	2068	2070	rBV2	77774	89844	2.17%	0.203%
36	14.515	2109	2113	2115	rBV4	30767	41964	1.01%	0.095%
37	14.545	2115	2118	2121	rVV	83805	87095	2.10%	0.197%
38	14.609	2125	2129	2137	rVB	2932575	2808584	67.79%	6.351%
39	14.768	2153	2156	2164	rVB	85022	141047	3.40%	0.319%
40	14.845	2165	2169	2172	rBV2	93428	111411	2.69%	0.252%
41	15.045	2200	2203	2208	rVB	55557	71154	1.72%	0.161%
42	15.098	2209	2212	2216	rVB	65347	76751	1.85%	0.174%
43	15.156	2217	2222	2235	rVB	1232557	1671007	40.33%	3.779%
44	15.574	2290	2293	2297	rVB3	56670	70538	1.70%	0.160%
45	15.768	2323	2326	2332	rBV8	26952	54234	1.31%	0.123%
46	16.486	2441	2448	2453	rBV2	34375	72085	1.74%	0.163%
47	16.827	2502	2506	2508	rBV5	29613	41468	1.00%	0.094%
48	16.874	2509	2514	2519	rVB3	35805	74505	1.80%	0.168%
49	18.280	2747	2753	2764	rVB3	35783	109562	2.64%	0.248%

Sum of corrected areas: 44220640

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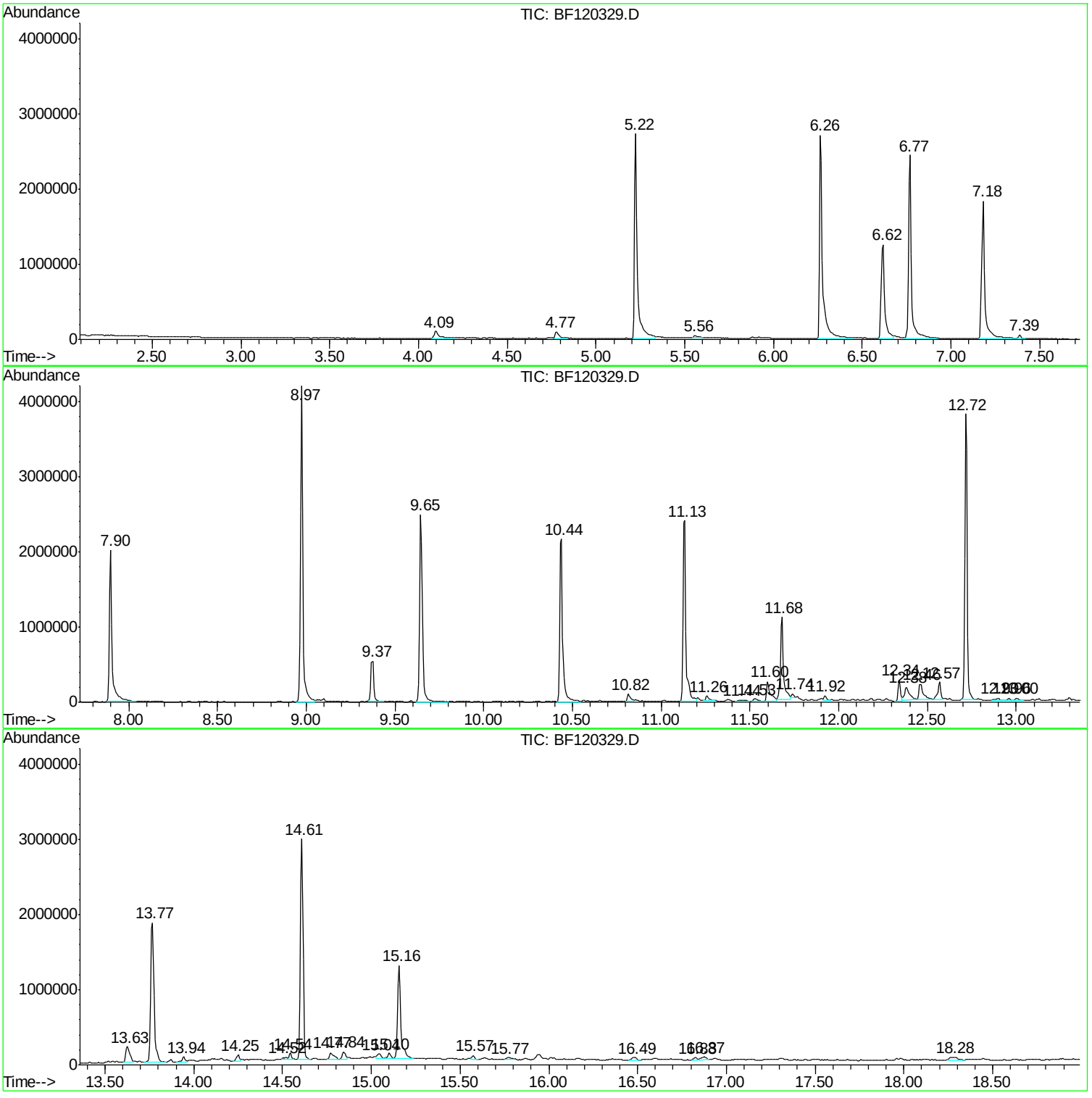
Instrument :
BNA_F
ClientSampleId :
TP-B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF120329.D
Acq On : 15 May 2020 18:47
Operator : MA/SJ
Sample : L2646-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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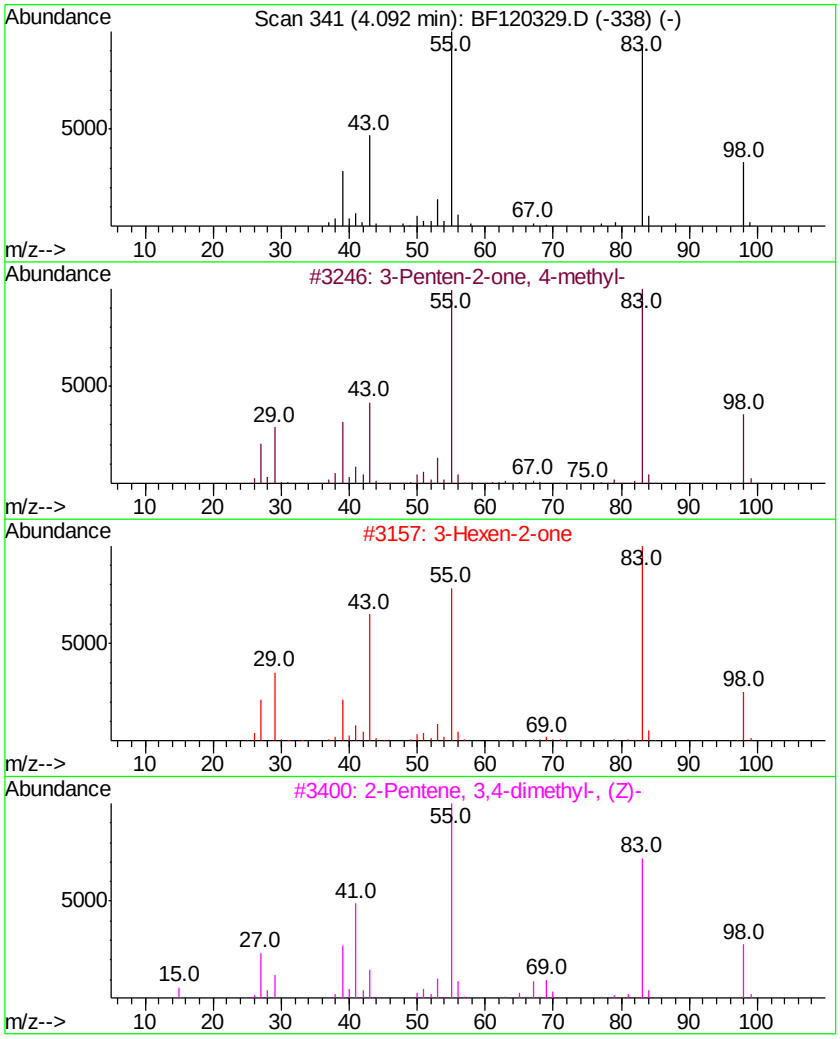
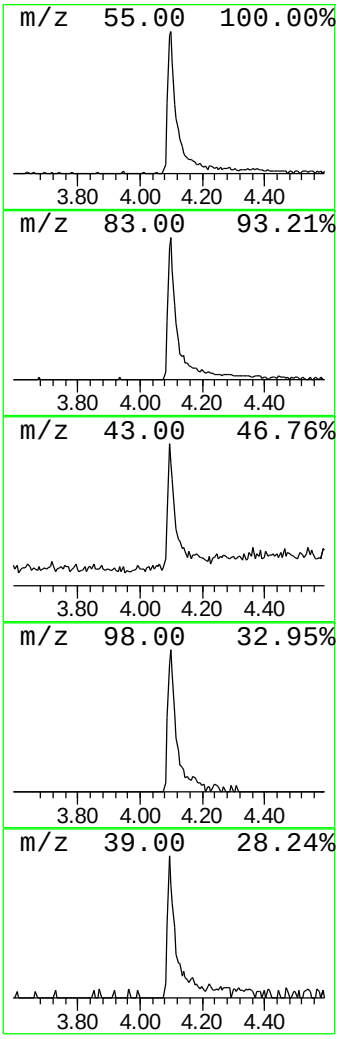
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.09	2.36 ng	192661	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
4	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78





Library Search Compound Report

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Data File : BF120329.D
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Operator : MA/SJ
Sample : L2646-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

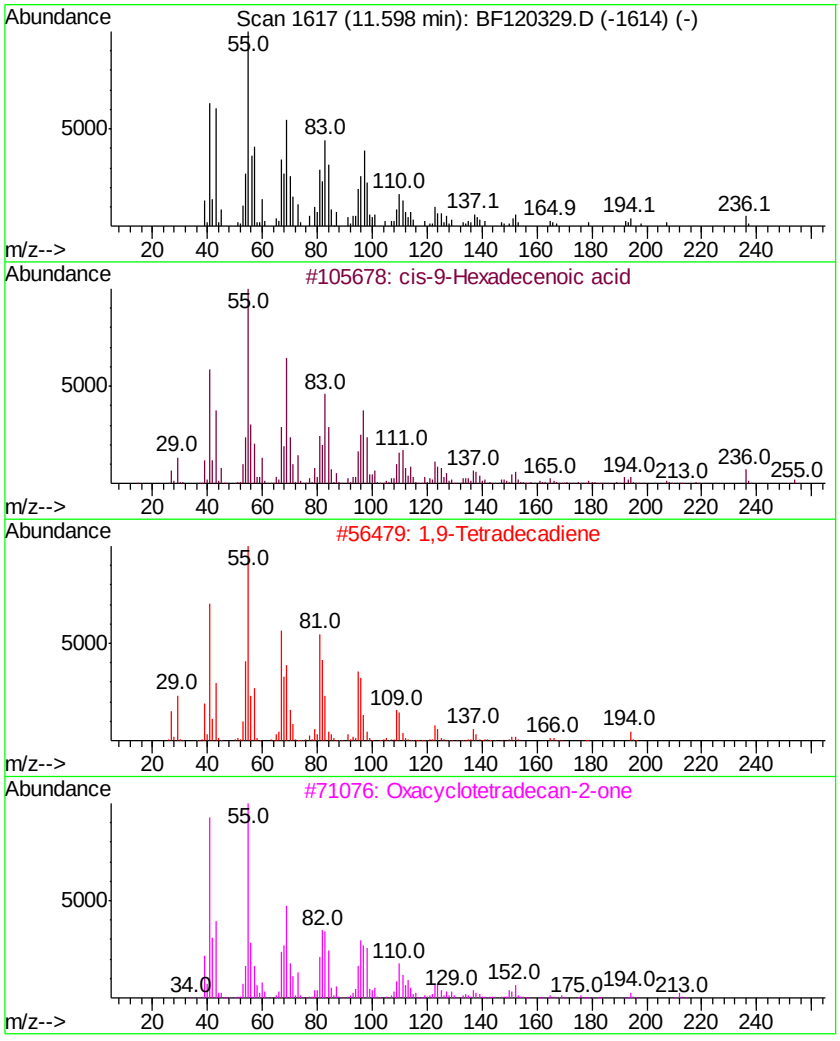
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

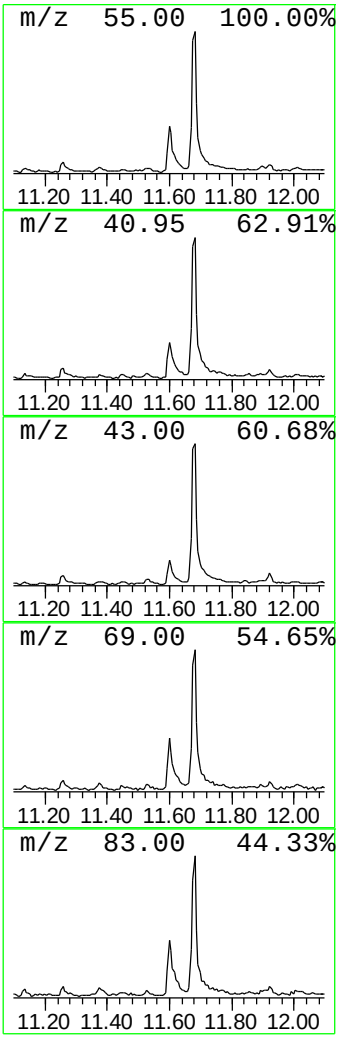
****

Peak Number 3 cis-9-Hexadecenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	2.90 ng	405733	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	91
2	1,9-Tetradecadiene	194	C14H26	112929-06-3	74
3	Oxacyclotetradecan-2-one	212	C13H24O2	001725-04-8	74
4	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	68
5	Palmitoleic acid	254	C16H30O2	000373-49-9	68





Library Search Compound Report

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Data File : BF120329.D
Acq On : 15 May 2020 18:47
Operator : MA/SJ
Sample : L2646-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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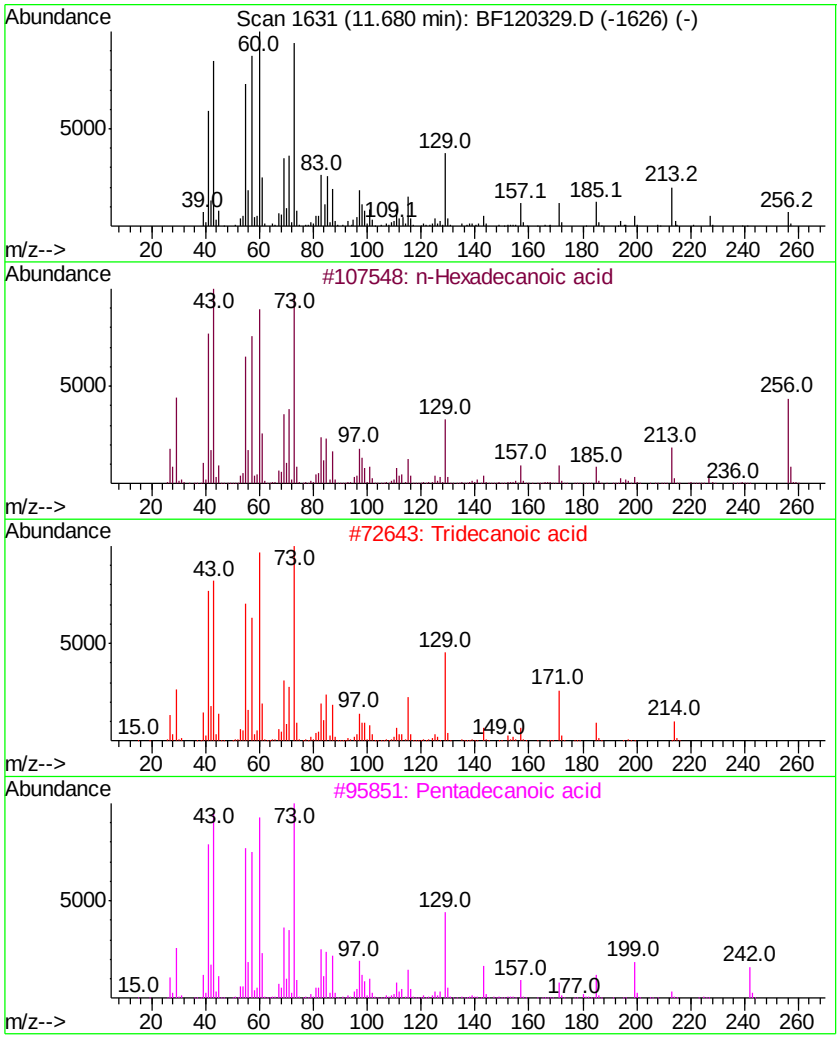
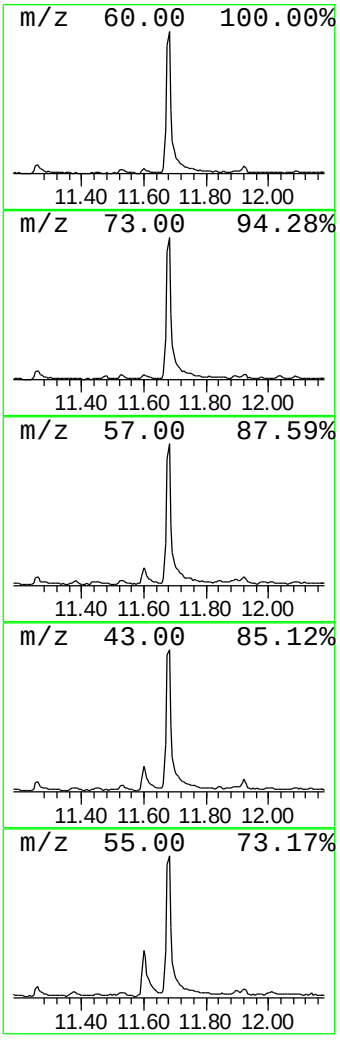
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	9.31 ng	1303520	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Library Search Compound Report

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Operator : MA/SJ
Sample : L2646-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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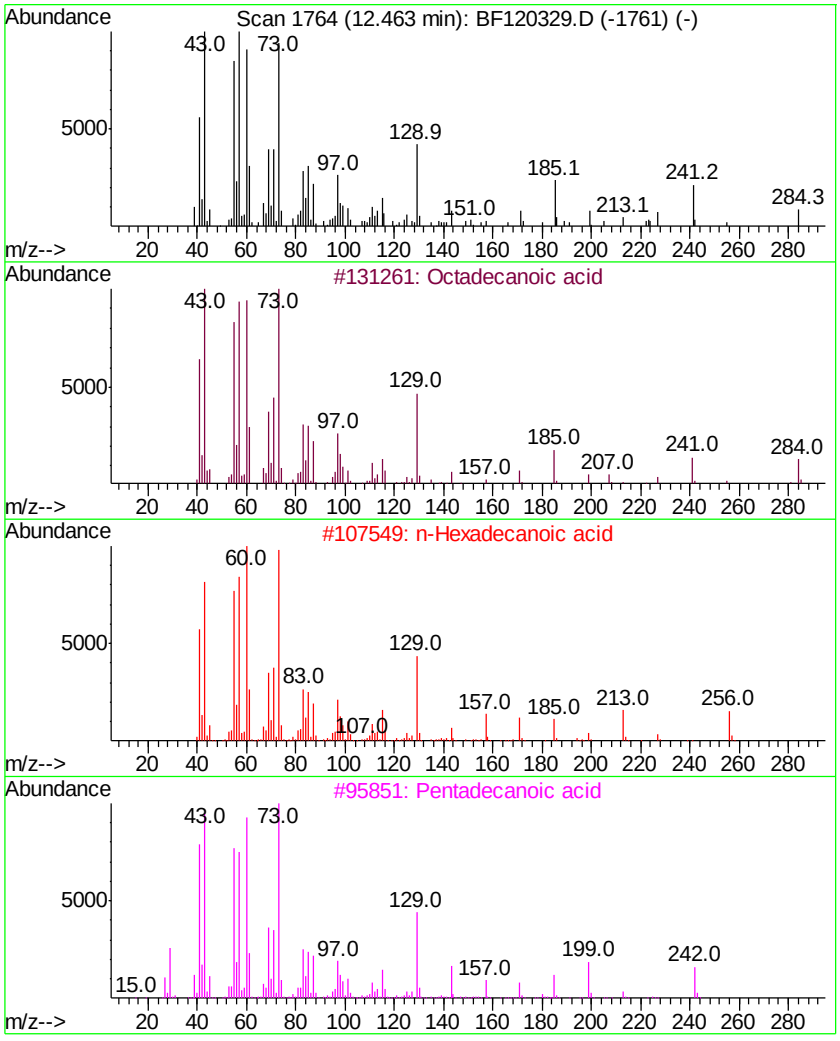
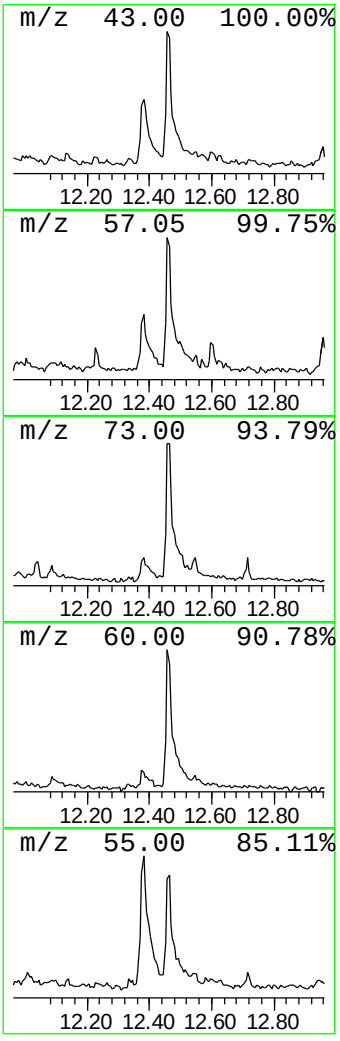
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	2.78 ng	316440	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Instrument : BNA_F
ClientSampleId : TP-B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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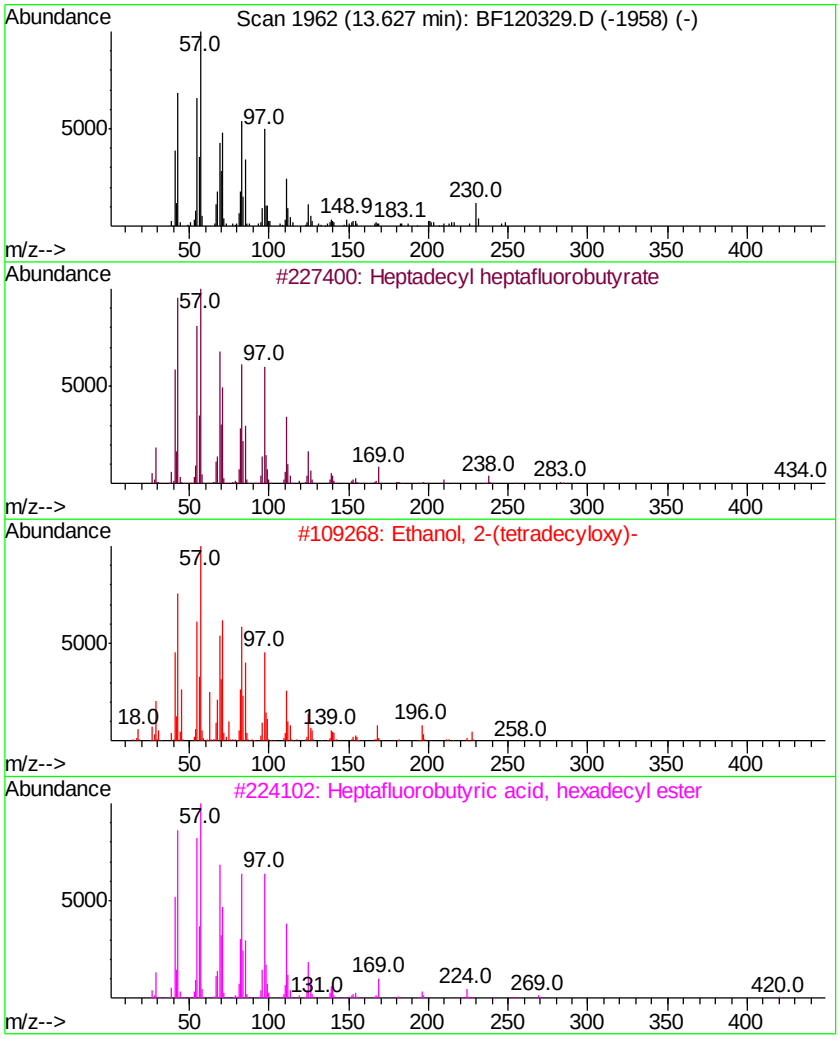
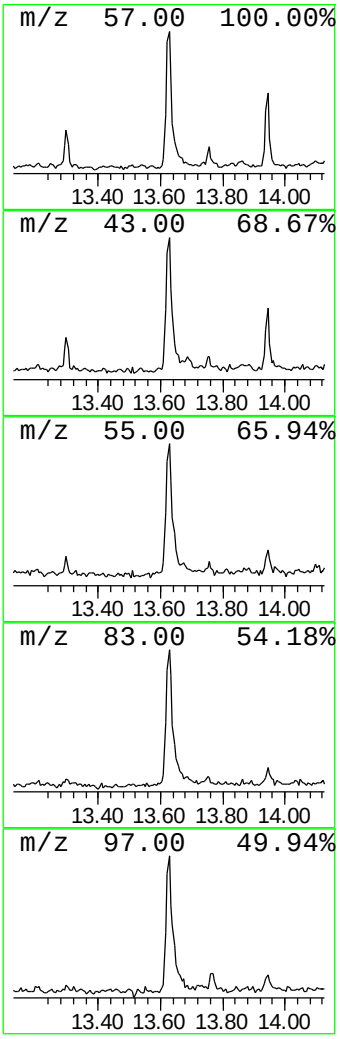
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.68 ng	305350	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	76
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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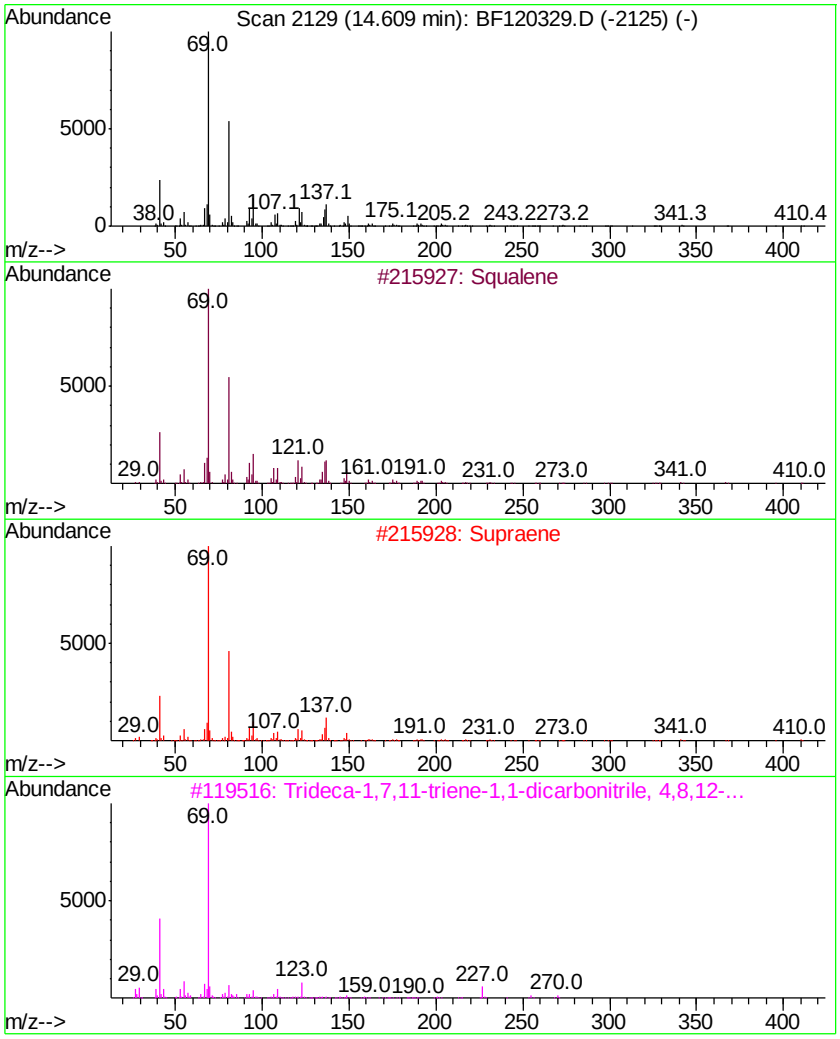
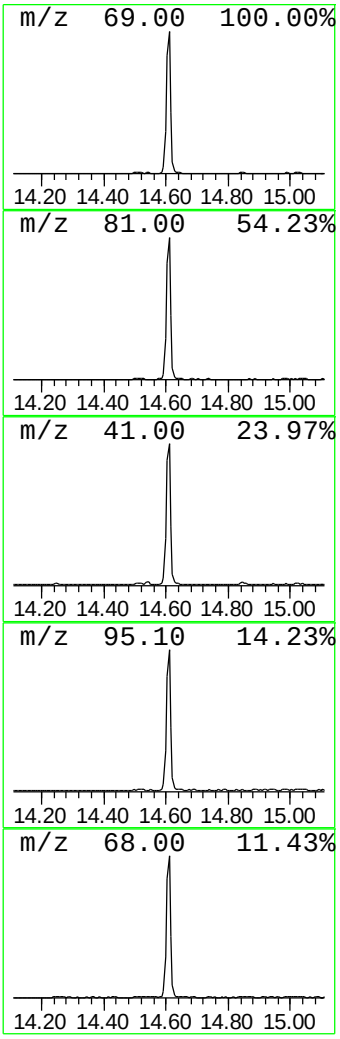
Peak Number 7 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	33.62 ng	2808580	Perylene-d12	15.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	98
2	Supraene	410	C30H50	007683-64-9	91
3	Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	53
4	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47
5	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	47





Tentatively Identified Compound (LSC) summary

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Operator : MA/SJ
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.09	2.4	ng	192661	1	6.62	1631830	20.0
cis-9-Hexadecenoi...	11.60	2.9	ng	405733	4	11.13	2800180	20.0
n-Hexadecanoic acid	11.68	9.3	ng	1303520	4	11.13	2800180	20.0
Octadecanoic acid	12.46	2.8	ng	316440	5	13.77	2275600	20.0
Heptadecyl heptaf...	13.63	2.7	ng	305350	5	13.77	2275600	20.0
Squalene	14.61	33.6	ng	2808580	6	15.16	1671010	20.0