LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110559.D
Acq On : 7 Nov 2018 17:00
Operator : JU/SJ
Sample : J5839-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-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-BF102318.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	2.251	24	28	45	rVB	200028	308732	21.96%	2.300%
2	4.575	420	423	435	rBV	30909	45871	3.26%	0.342%
3	5.175	522	525	539	rBV	96412	115673	8.23%	0.862%
4	5.569	588	592	610	rBV	896301	846841	60.25%	6.308%
5	6.569	758	762	783	rBV	1051861	1134367	80.70%	8.450%
6	6.716	783	787	791	rBV	1259359	1072035	76.27%	7.985%
7	6.951	823	827	833	rBV	467873	429391	30.55%	3.198%
8	7.104	849	853	866	rBV	1011288	872013	62.04%	6.495%
9	7.510	918	922	940	rBV	680254	698725	49.71%	5.205%
10	8.233	1041	1045	1060	rBV	544914	577925	41.12%	4.305%
11	9.304	1223	1227	1238	rBV	1523773	1405629	100.00%	10.470%
12	9.698	1291	1294	1302	rBV	139741	141004	10.03%	1.050%
13	9.992	1340	1344	1355	rBV	746942	681866	48.51%	5.079%
14	10.786	1475	1479	1488	rBV	476272	512694	36.47%	3.819%
15	11.486	1594	1598	1607	rBV	706495	673682	47.93%	5.018%
16	11.986	1680	1683	1688	rBV3	22716	29796	2.12%	0.222%
17	12.774	1813	1817	1822	rBV4	20614	34687	2.47%	0.258%
18	13.068	1863	1867	1870	rBV	1284162	1178618	83.85%	8.779%
19	13.615	1957	1960	1963	rBV2	21496	25490	1.81%	0.190%
20	13.945	2012	2016	2023	rBV	75619	93418	6.65%	0.696%
21	14.080	2034	2039	2044	rVB	98408	100552	7.15%	0.749%
22	14.133	2044	2048	2057	rBV	451737	485407	34.53%	3.616%
23	14.257	2066	2069	2075	rVB	68695	74665	5.31%	0.556%
24	14.562	2118	2121	2127	rBV	151541	153360	10.91%	1.142%
25	14.880	2170	2175	2180	rBV	259532	295831	21.05%	2.204%
26	15.233	2230	2235	2243	rVB	258873	325995	23.19%	2.428%
27	15.627	2297	2302	2305	rBV	213425	303032	21.56%	2.257%
28	15.662	2305	2308	2316	rVB	310013	422449	30.05%	3.147%
29	16.086	2374	2380	2385	rVB	140155	220687	15.70%	1.644%
30	16.609	2465	2469	2480	rVB2	69500	123457	8.78%	0.920%
31	17.233	2573	2575	2583	rVB2	25699	41021	2.92%	0.306%

Sum of corrected areas: 13424913

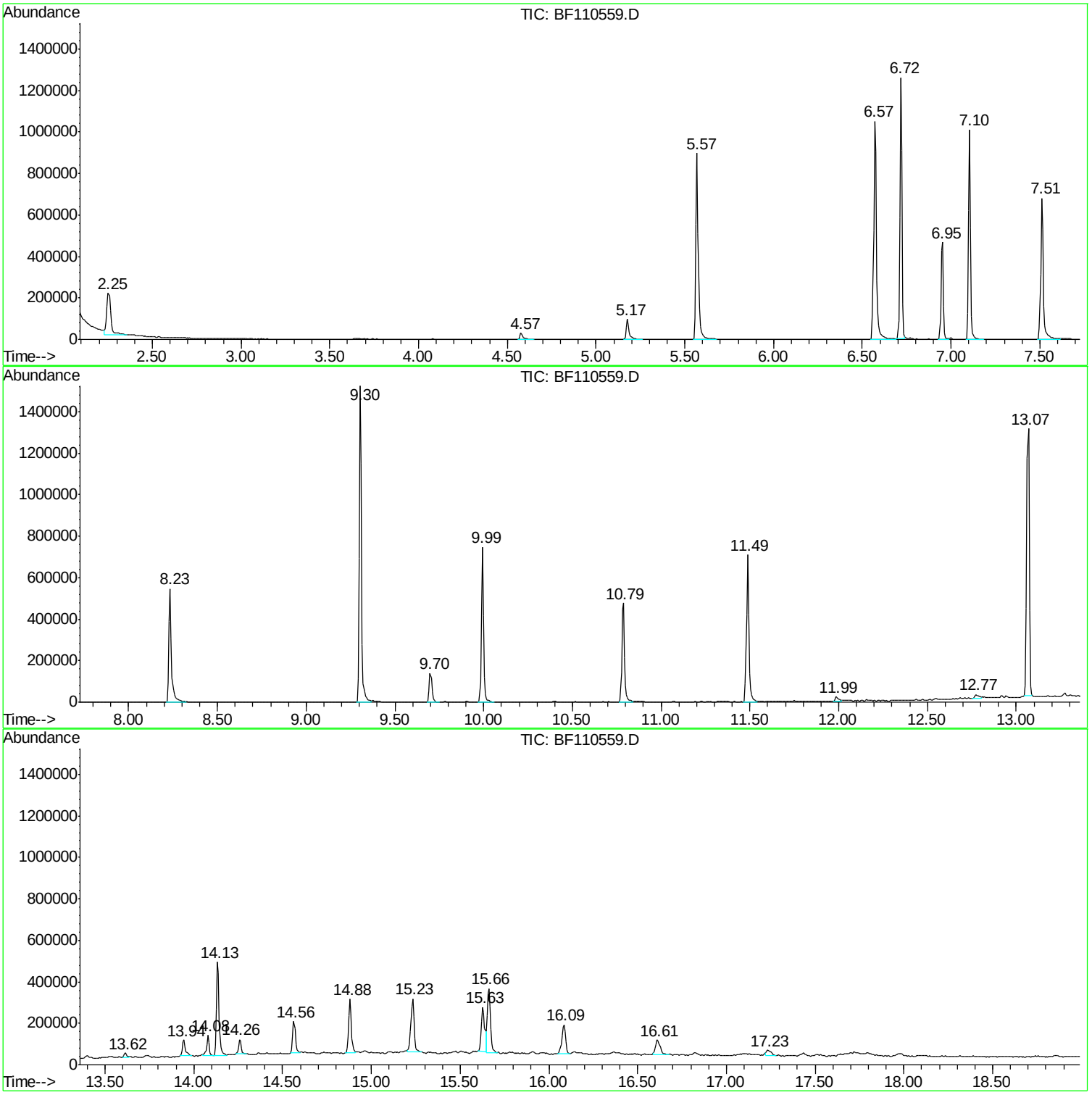
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110718\
Data File : BF110559.D
Acq On : 7 Nov 2018 17:00
Operator : JU/SJ
Sample : J5839-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

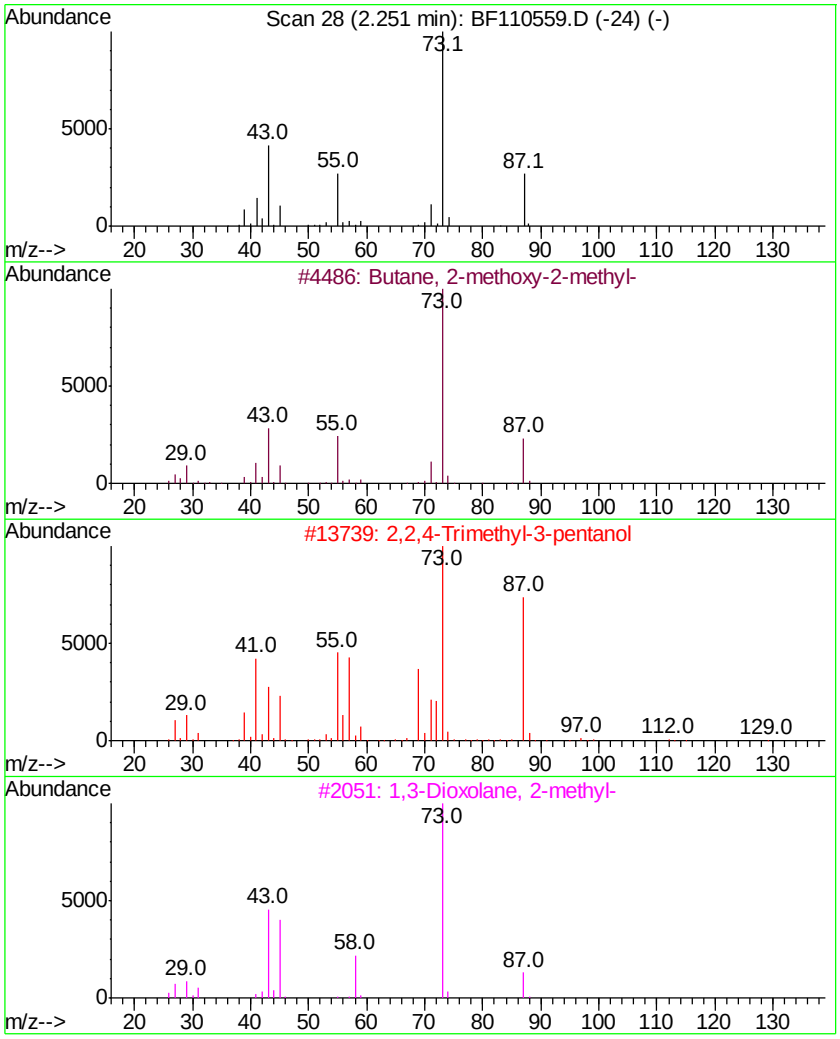
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

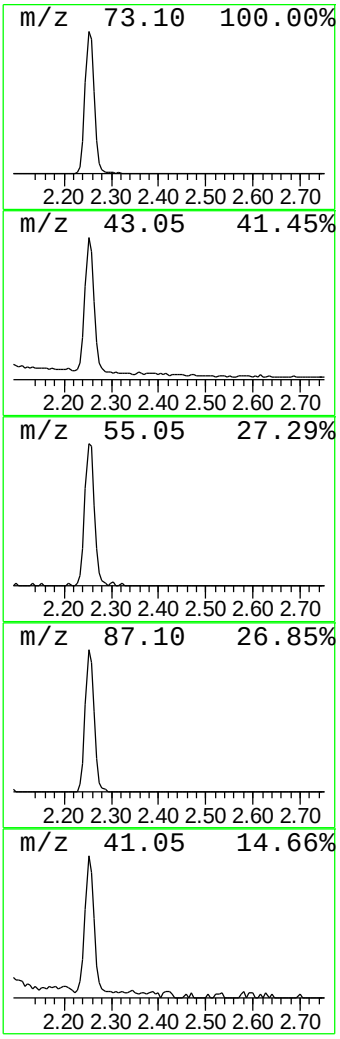
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	14.38 ng	308732	1,4-Dichlorobenzene-d4	6.95

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Sample : J5839-11
Misc :
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Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

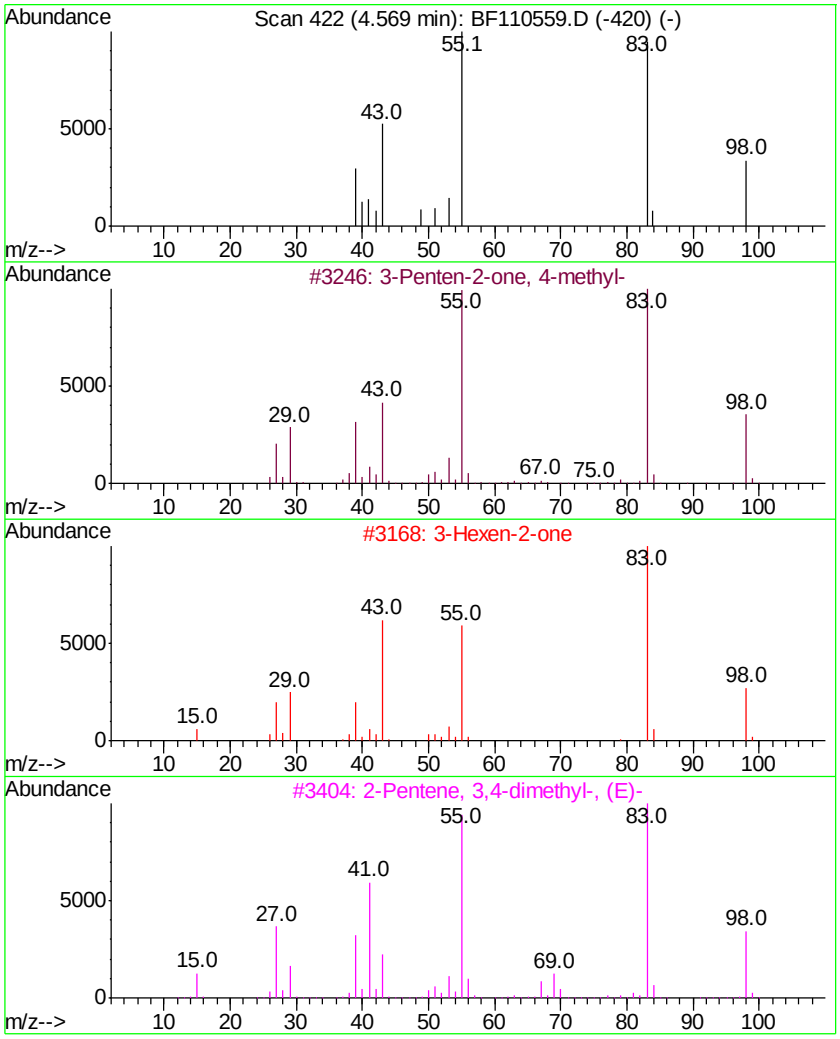
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

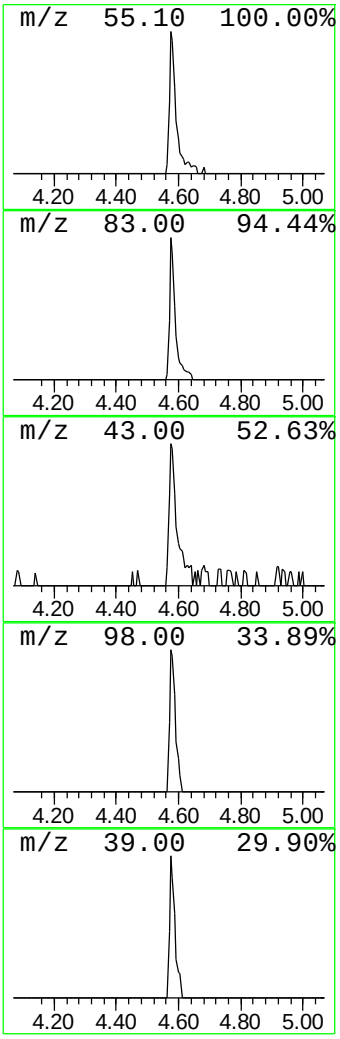
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	2.14 ng	45871	1,4-Dichlorobenzene-d4	6.95

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-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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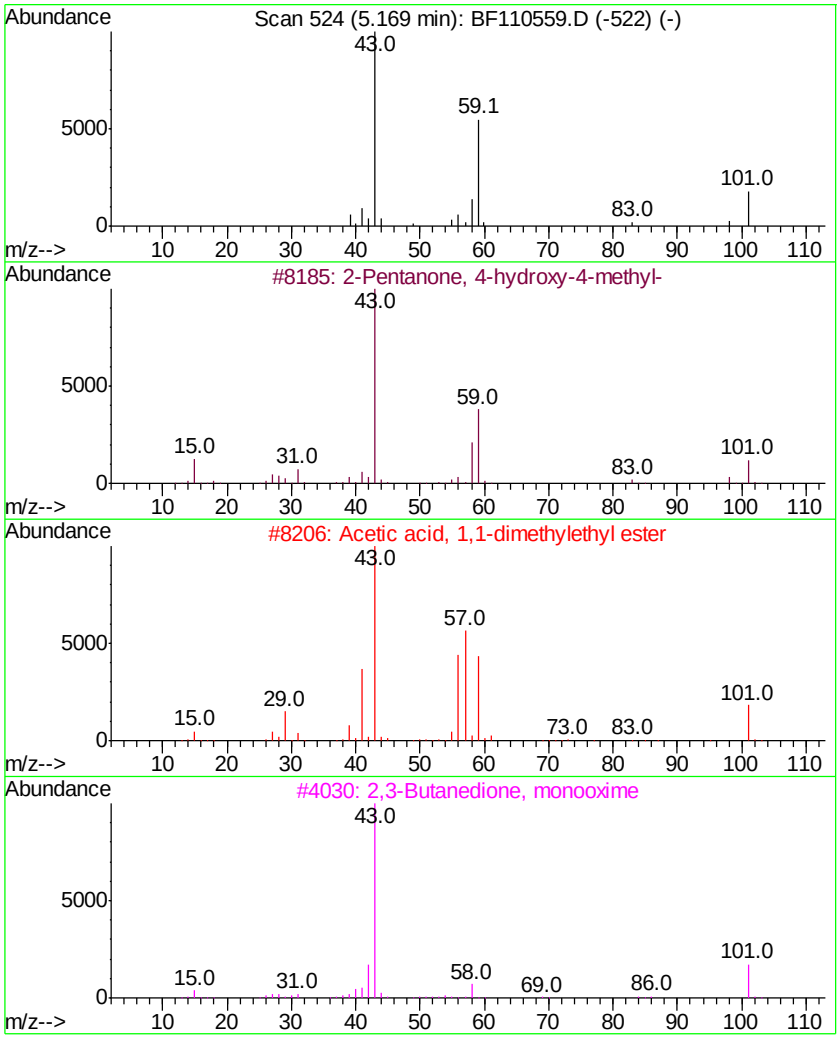
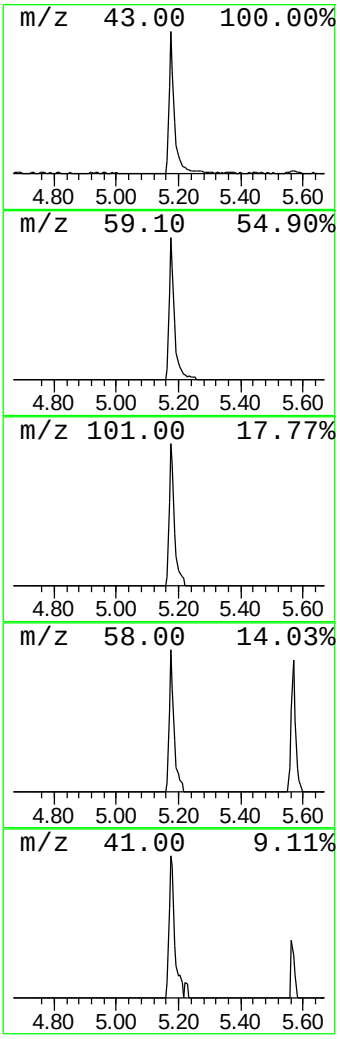
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	5.39 ng	115673	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	3-Hexanol	102	C6H14O	000623-37-0	9
5	3-Octanol	130	C8H18O	000589-98-0	9





Library Search Compound Report

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Sample : J5839-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

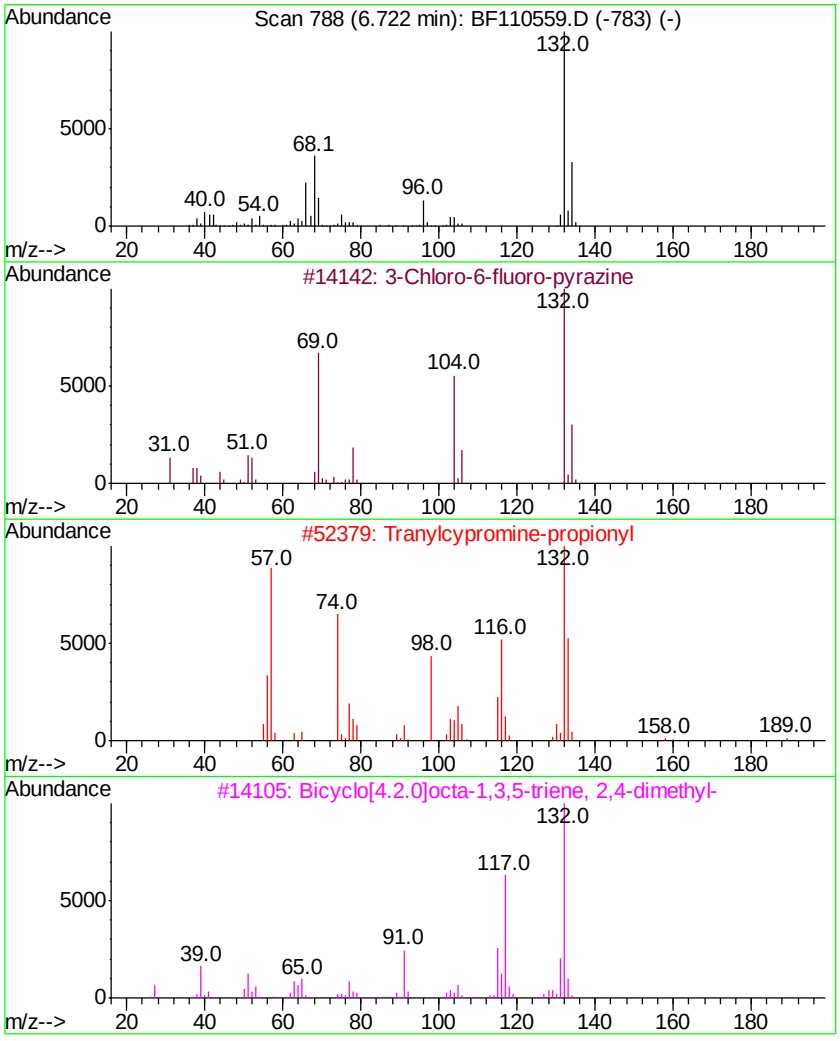
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

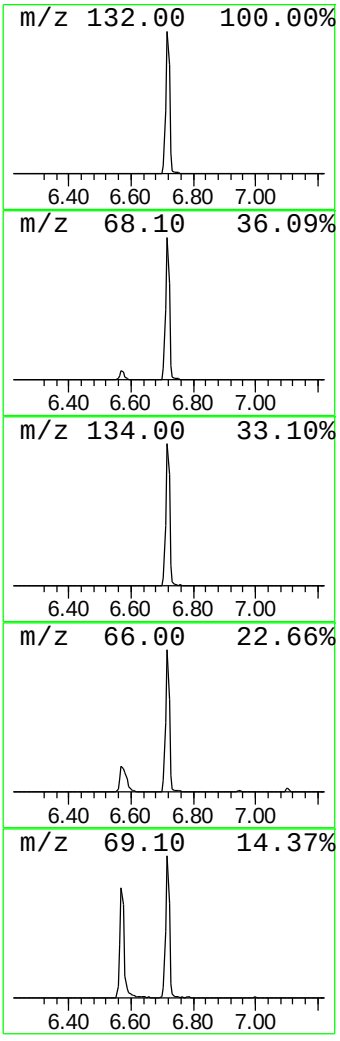
****

Peak Number 4 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	49.93 ng	1072040	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1-Aminoindan	133	C9H11N	034698-41-4	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-7-S

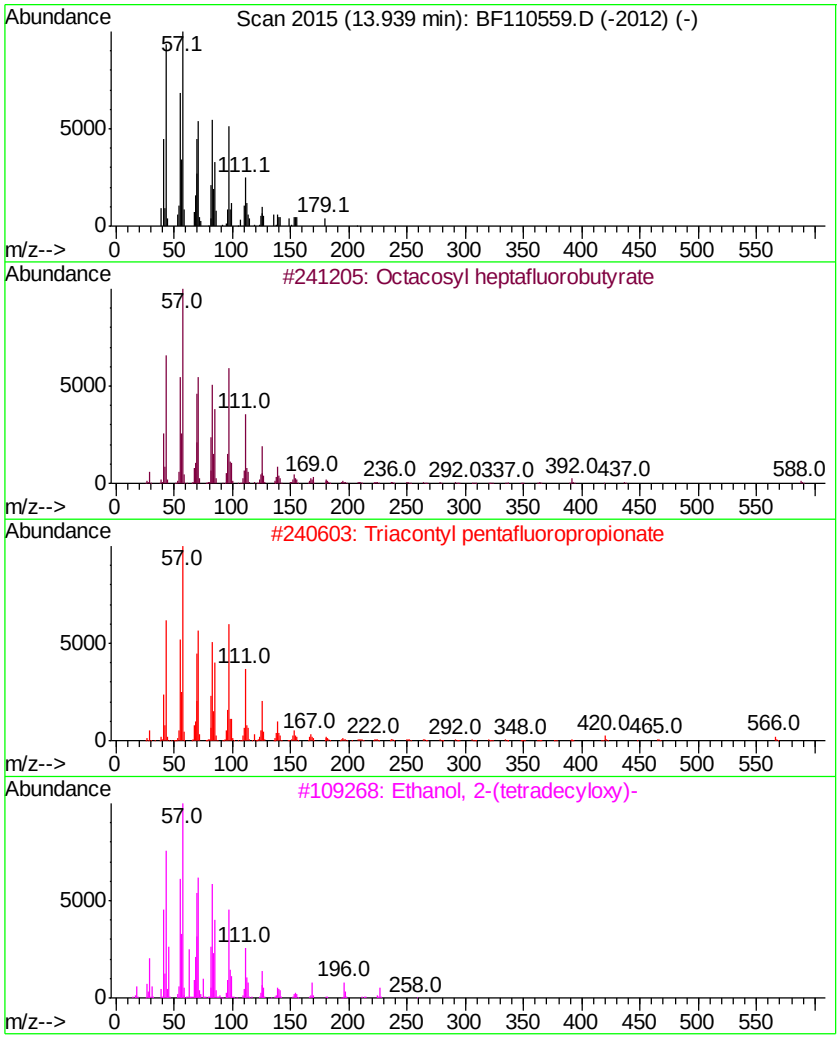
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

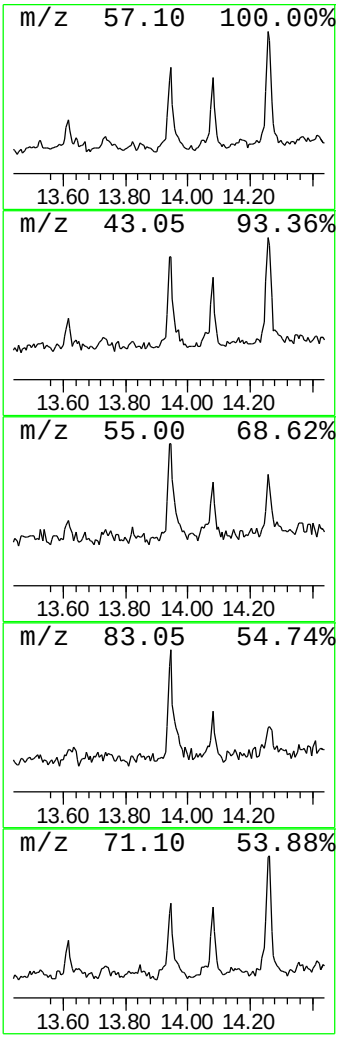
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octacosyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.85 ng	93418	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91
2	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : SB-7-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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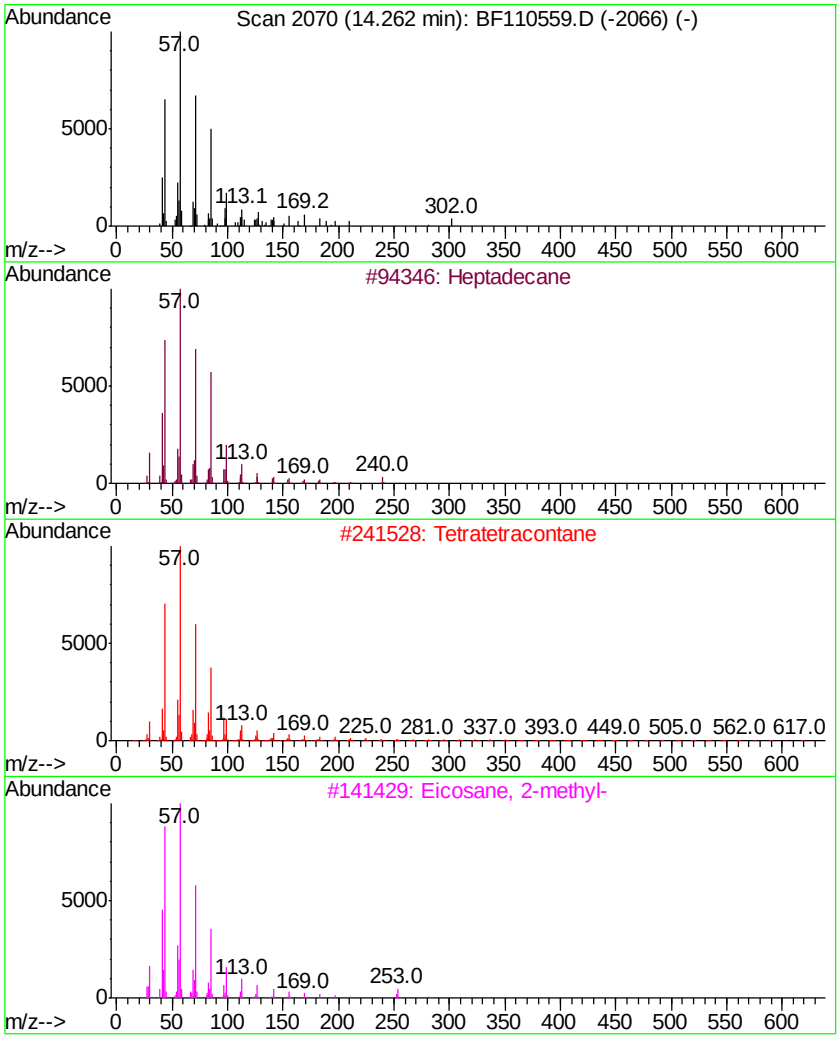
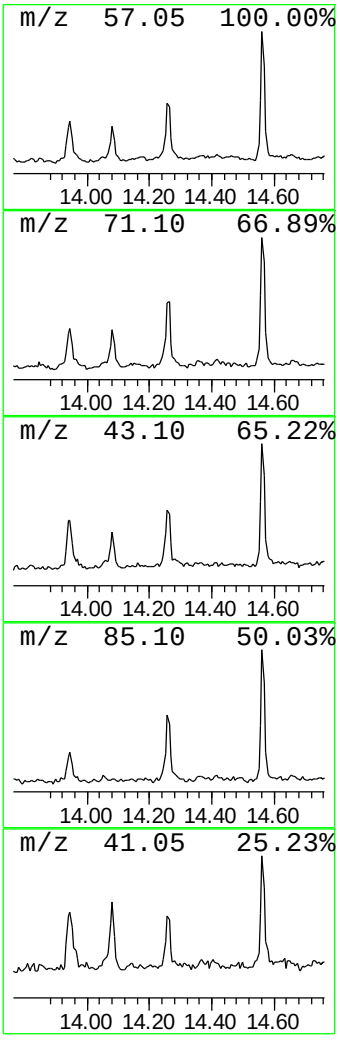
****

Peak Number 7 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	3.08 ng	74665	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Tetratetracontane	619	C44H90	007098-22-8	80
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	72
4	Heneicosane	296	C21H44	000629-94-7	68
5	Hexacosane	366	C26H54	000630-01-3	68





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

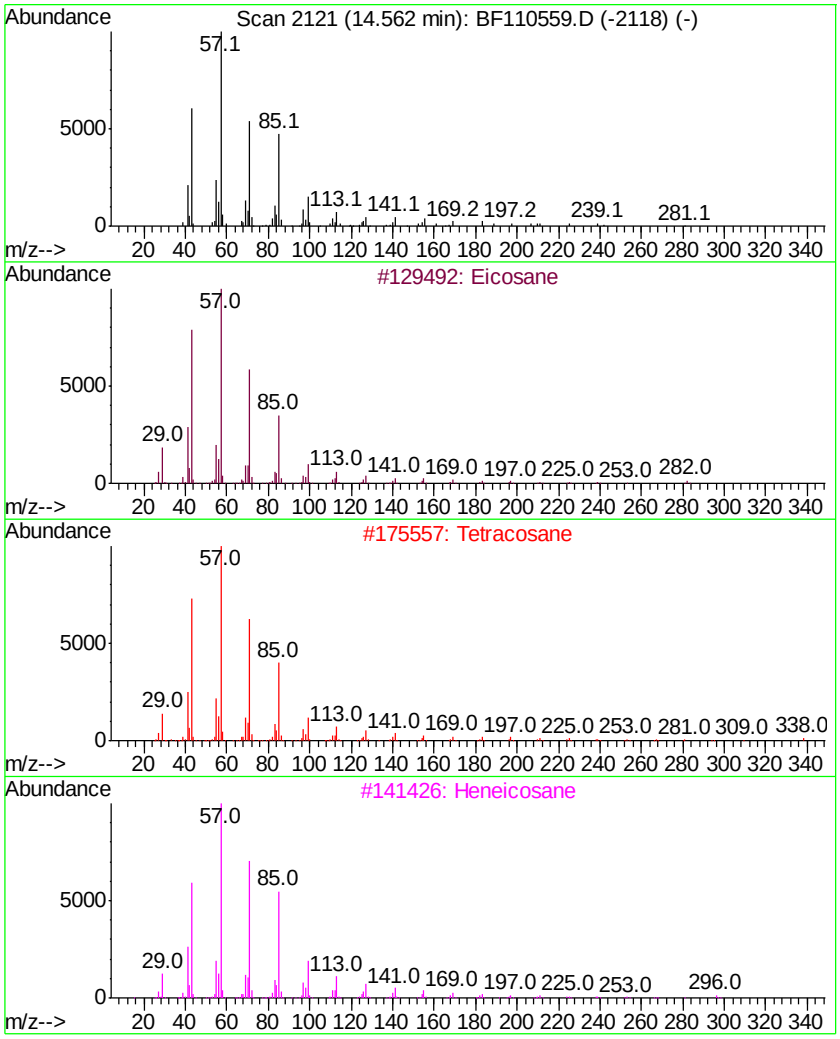
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

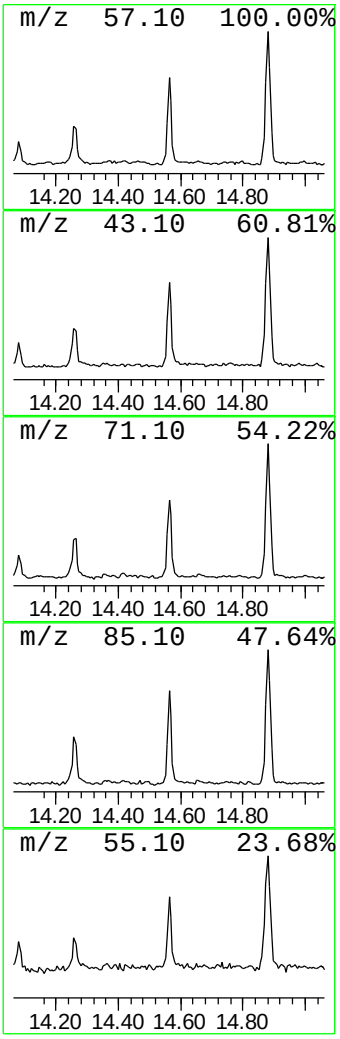
****

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	6.32 ng	153360	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
5	Octacosane	394	C28H58	000630-02-4	81





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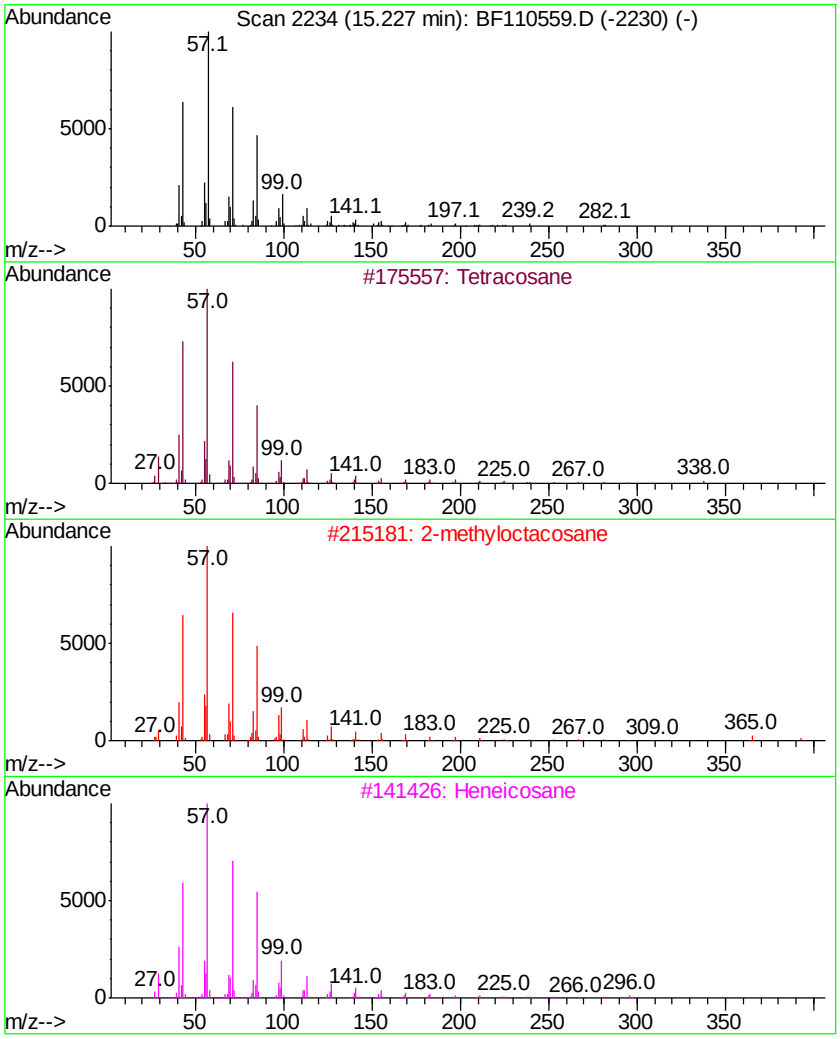
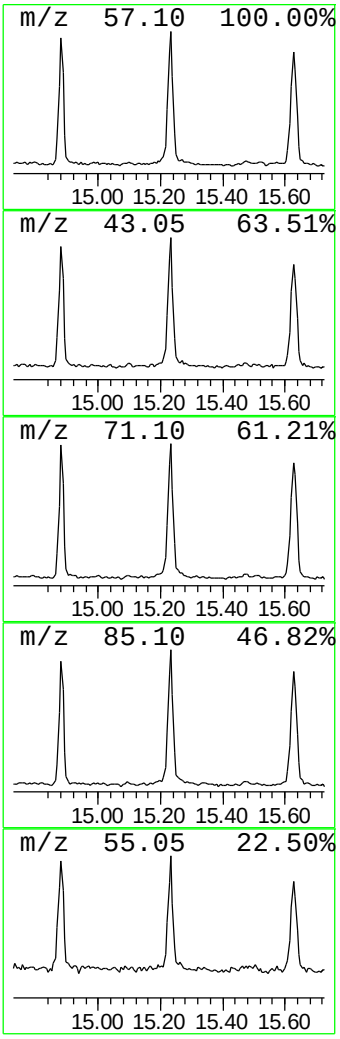
****

Peak Number 10 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	15.43 ng	325995	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Octadecane	254	C18H38	000593-45-3	87





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

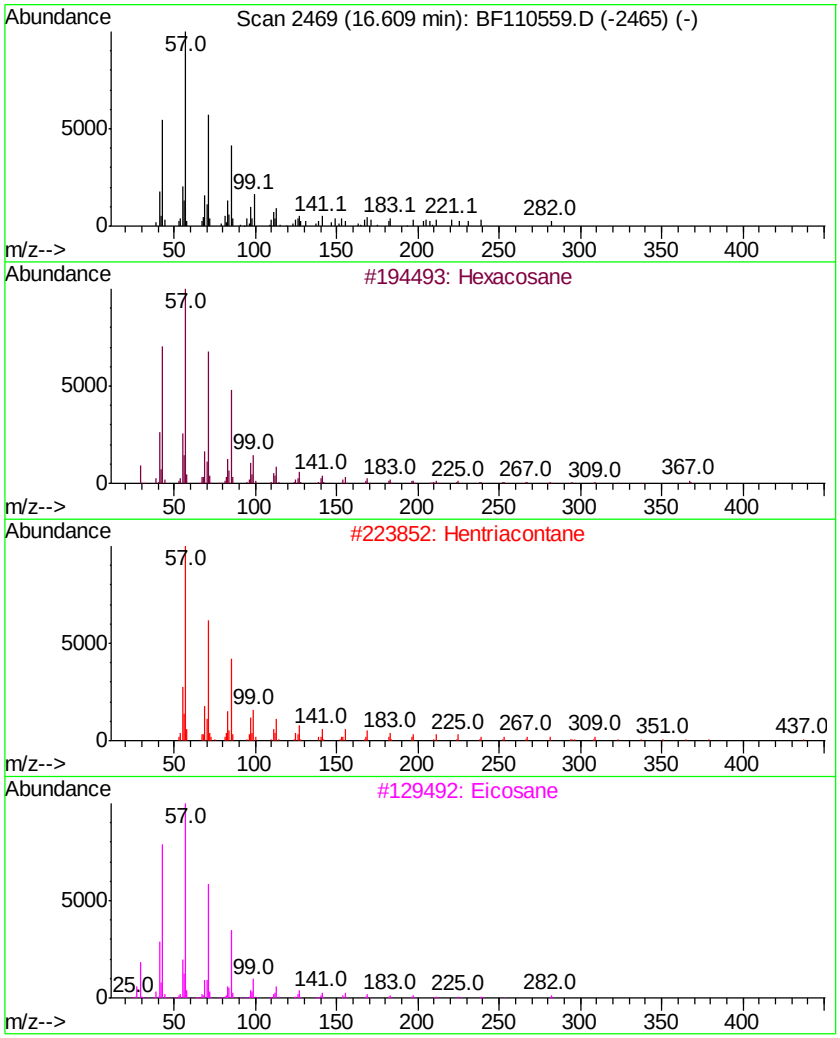
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

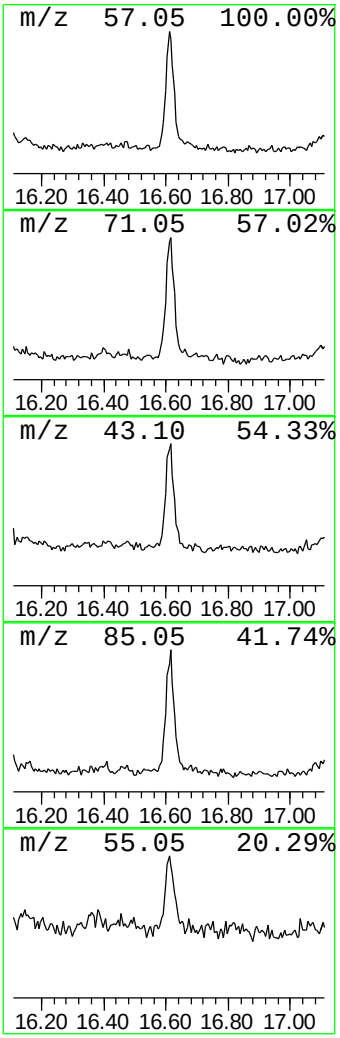
****

Peak Number 12 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	5.84 ng	123457	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Eicosane	282	C20H42	000112-95-8	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Octacosane	394	C28H58	000630-02-4	87





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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
Butane, 2-methoxy...	2.25	14.4	ng	308732	1	6.95	429391	20.0
3-Penten-2-one, 4...	4.57	2.1	ng	45871	1	6.95	429391	20.0
2-Pentanone, 4-hy...	5.17	5.4	ng	115673	1	6.95	429391	20.0
unknown6.72	6.72	49.9	ng	1072040	1	6.95	429391	20.0
Octacosyl heptafl...	13.94	3.9	ng	93418	5	14.13	485407	20.0
Heptadecane	14.26	3.1	ng	74665	5	14.13	485407	20.0
Eicosane	14.56	6.3	ng	153360	5	14.13	485407	20.0
Tetracosane	15.23	15.4	ng	325995	6	15.66	422449	20.0
Hexacosane	16.61	5.8	ng	123457	6	15.66	422449	20.0