LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061319\
Data File : BF115000.D
Acq On : 13 Jun 2019 13:51
Operator : HP/JU
Sample : K3294-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2(0-5)

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-BF061219.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	2.975	149	151	166	rBV	61538	147330	1.85%	0.328%
2	3.163	177	183	193	rVB	64702	127832	1.60%	0.285%
3	4.181	348	356	359	rBV	3762737	5332975	66.90%	11.887%
4	4.857	460	471	474	rBV	4003799	7971612	100.00%	17.769%
5	5.251	535	538	547	rBV	468695	438232	5.50%	0.977%
6	6.287	709	714	717	rBV	3023045	2648933	33.23%	5.904%
7	6.410	732	735	739	rBV	1200291	1049720	13.17%	2.340%
8	6.645	771	775	779	rBV	1948706	1561934	19.59%	3.482%
9	6.804	798	802	805	rBV	4294181	3664810	45.97%	8.169%
10	6.969	827	830	838	rVB	117641	98581	1.24%	0.220%
11	7.210	866	871	874	rBV	3037504	2746752	34.46%	6.122%
12	7.928	989	993	996	rBV	2486523	2002853	25.12%	4.464%
13	9.004	1171	1176	1179	rBV	6013955	5182020	65.01%	11.551%
14	9.398	1239	1243	1246	rBV	1071809	865905	10.86%	1.930%
15	9.675	1286	1290	1294	rBV	2540586	2115958	26.54%	4.716%
16	11.145	1536	1540	1544	rBV	1955847	1755421	22.02%	3.913%
17	12.727	1805	1809	1813	rBV	4017813	3550629	44.54%	7.914%
18	13.639	1961	1964	1972	rBV2	173530	281792	3.53%	0.628%
19	13.768	1982	1986	1990	rBV	1597794	1456817	18.28%	3.247%
20	14.527	2112	2115	2118	rBV	337885	364714	4.58%	0.813%
21	15.145	2216	2220	2225	rBV	1215856	1340692	16.82%	2.988%
22	16.609	2466	2469	2476	rVB6	88613	157891	1.98%	0.352%

Sum of corrected areas: 44863403

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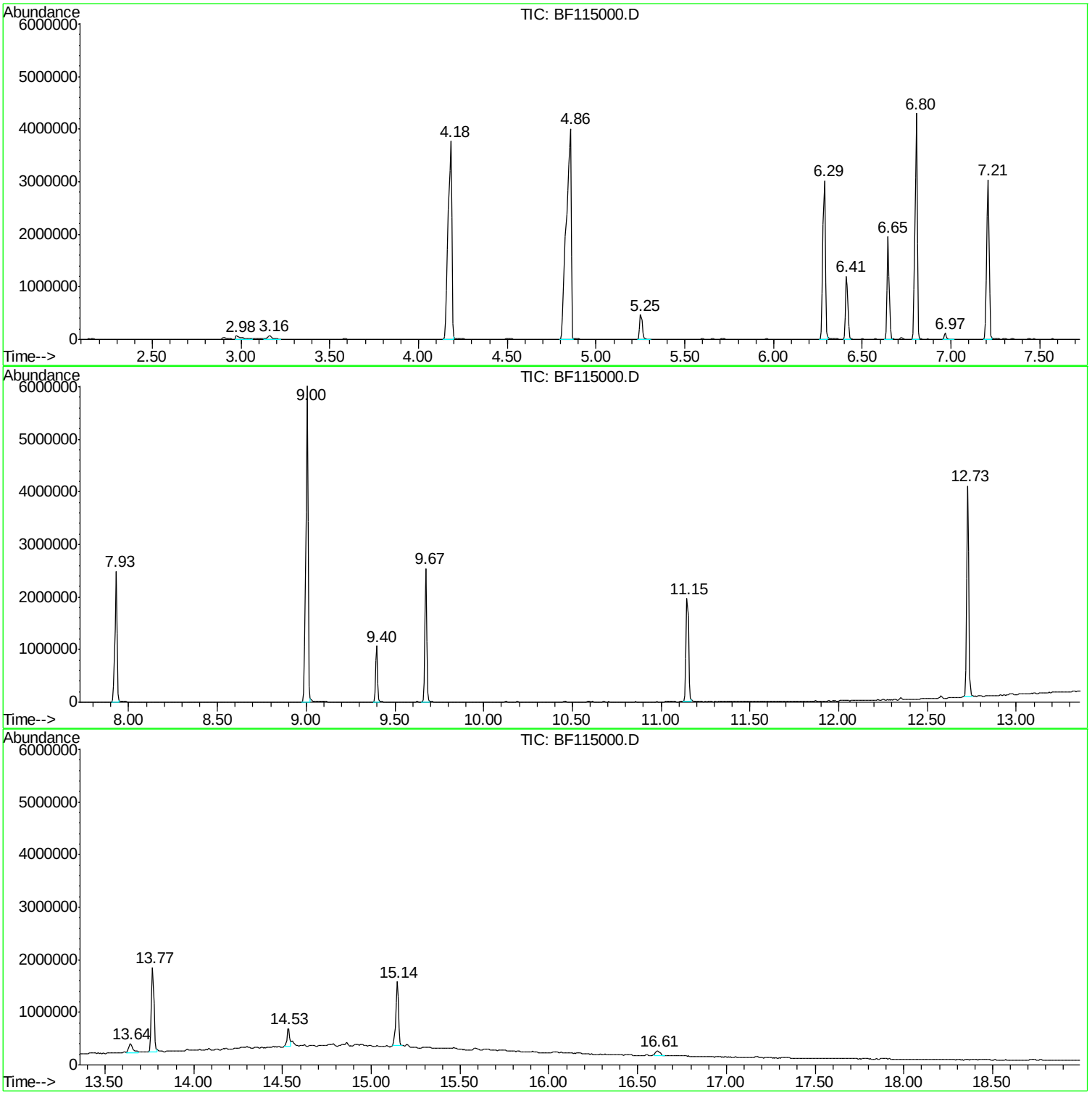
BNA_F
ClientSampleId :
S2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.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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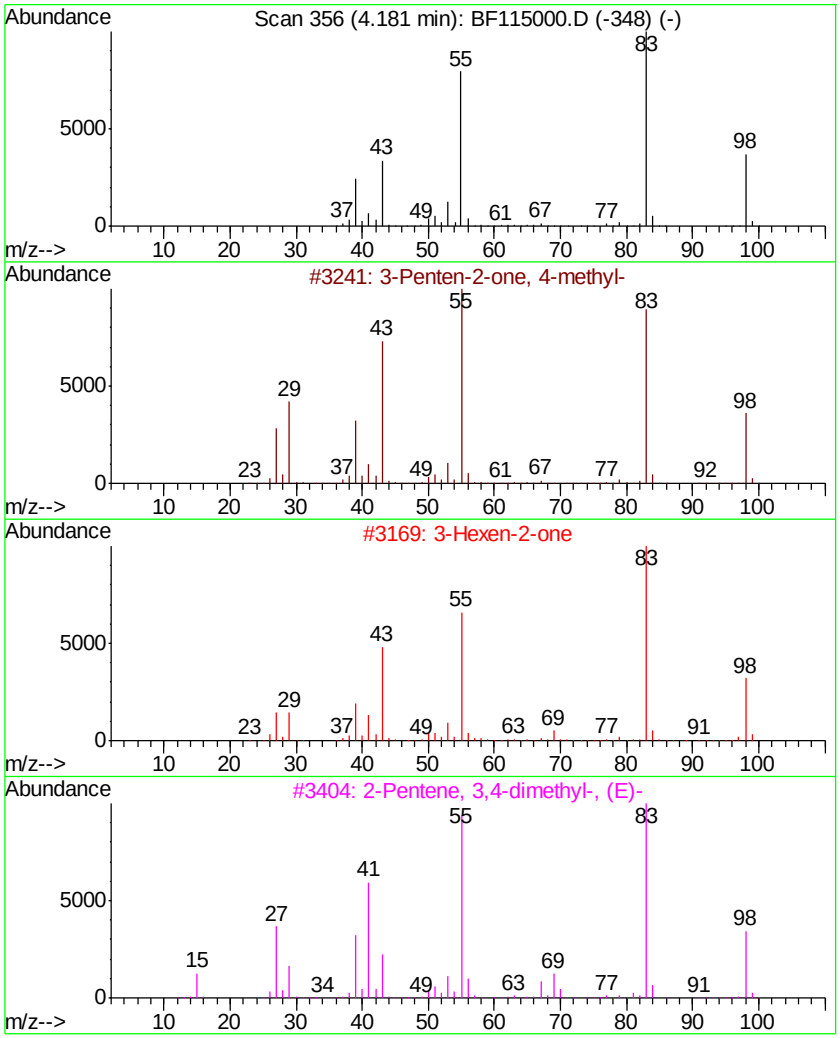
TIC Integration Parameters: LSCINT.P

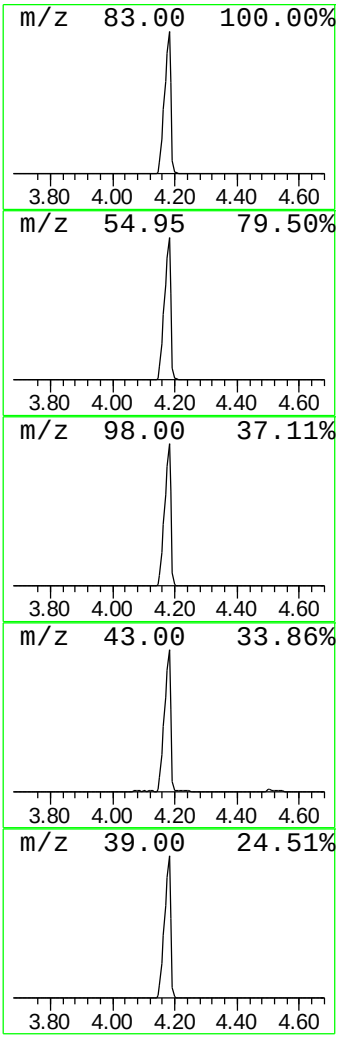
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	68.29 ng	5332980	1,4-Dichlorobenzene-d4	6.65

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	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : S2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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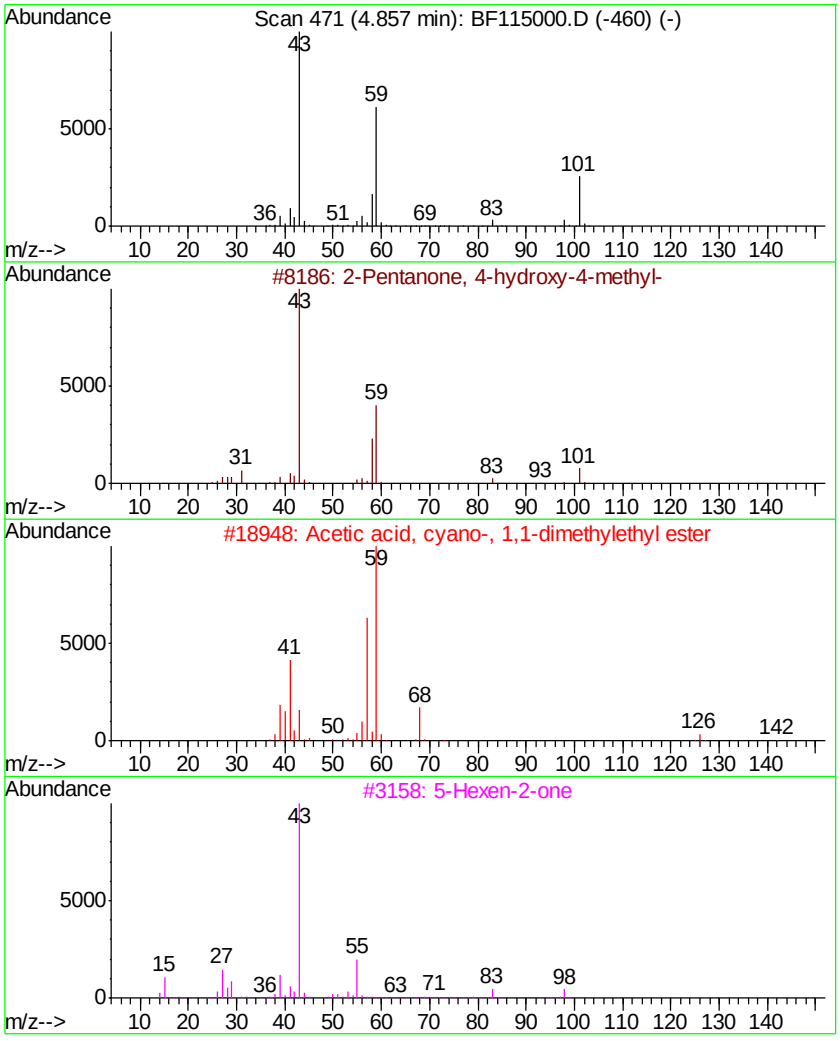
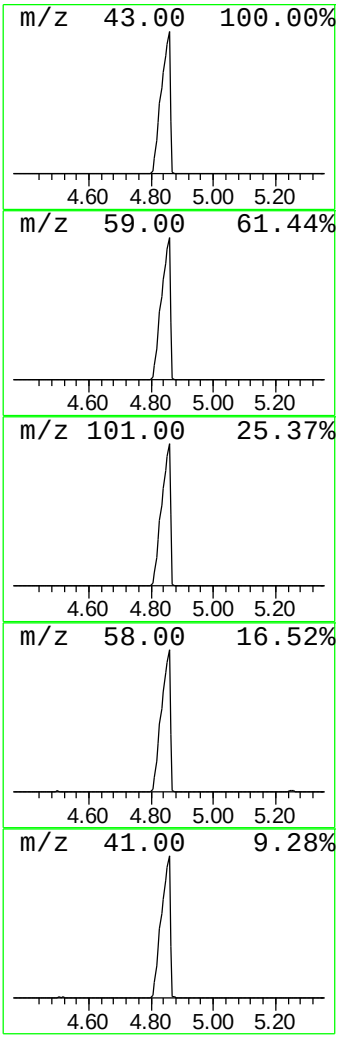
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	102.07 ng	7971610	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : HP/JU
Sample : K3294-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.M
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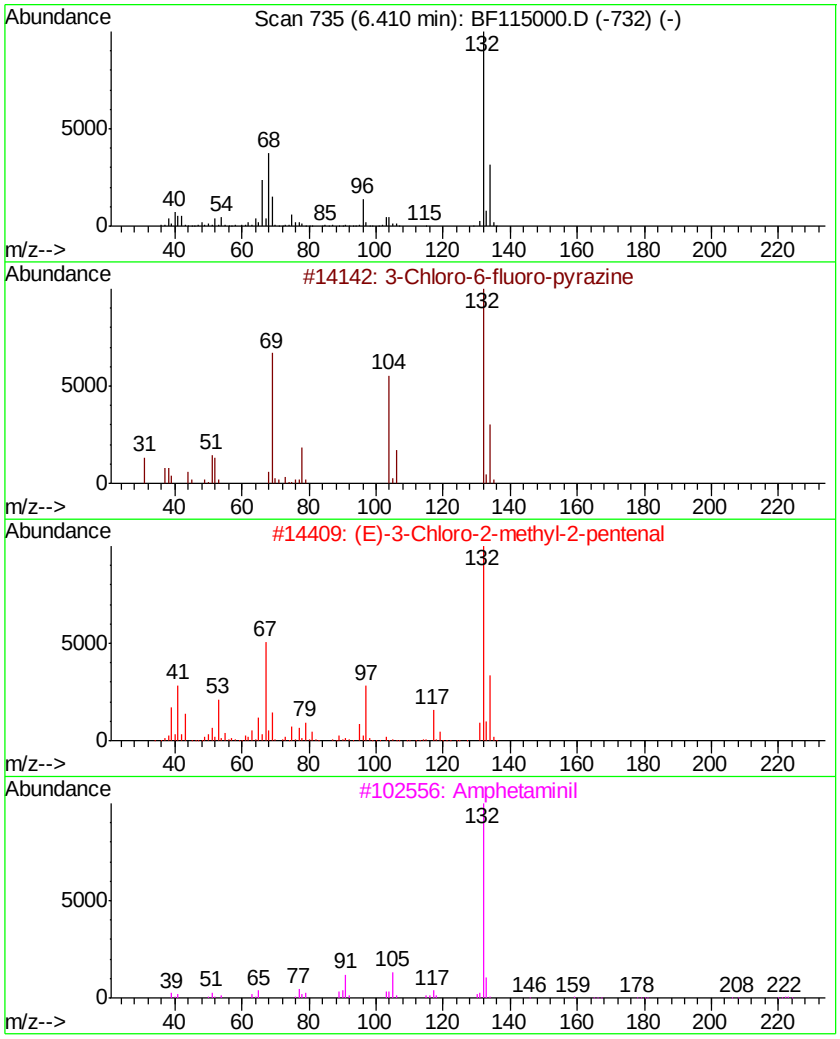
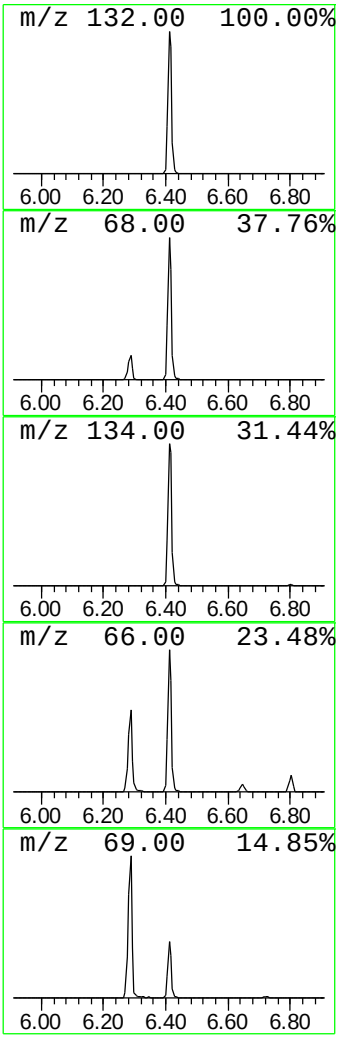
Peak Number 3 unknown6.41 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	13.44 ng	1049720	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : S2(0-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.M
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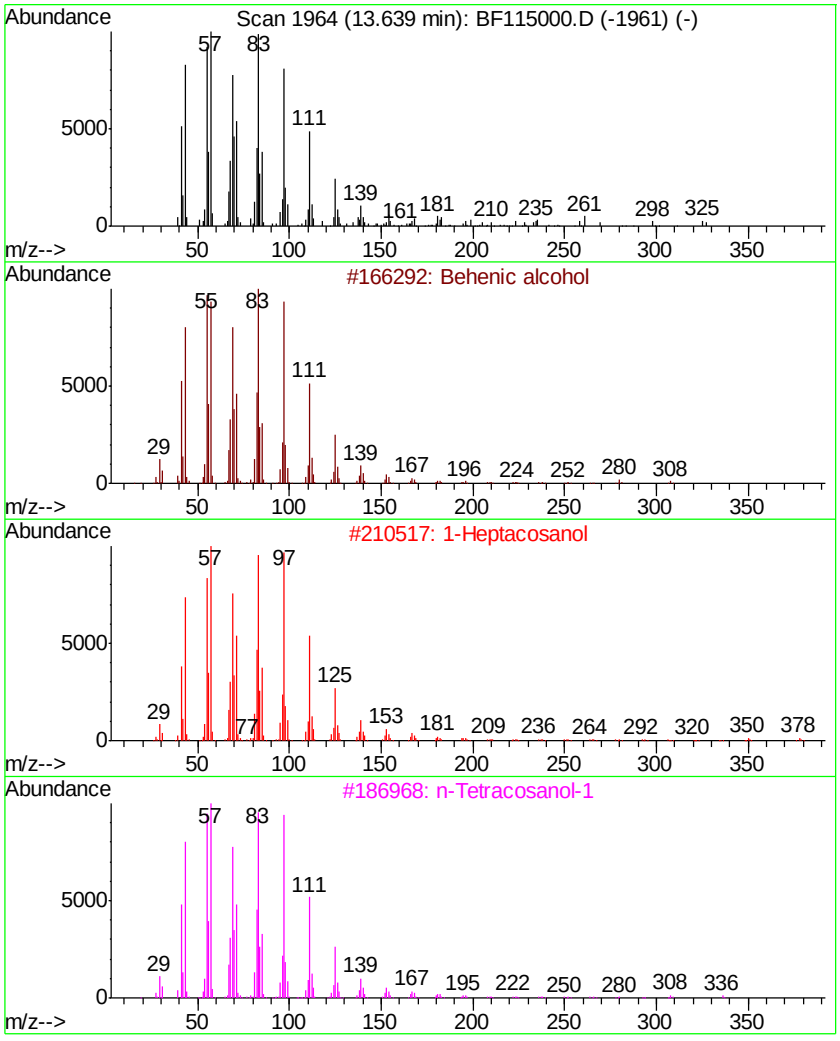
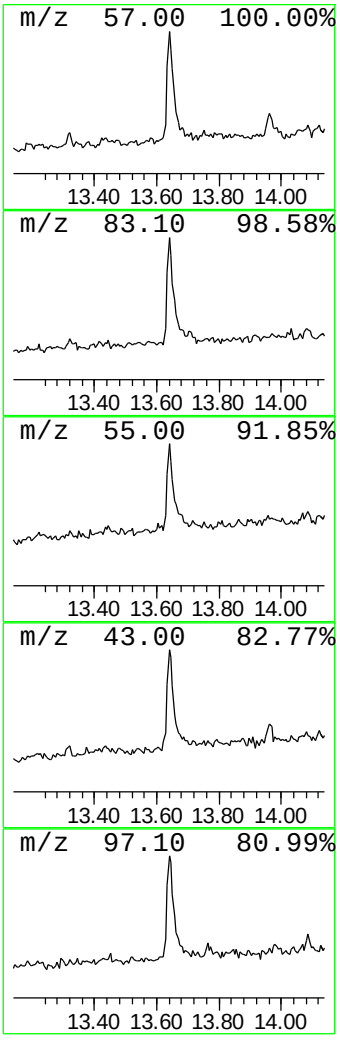
Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	3.87 ng	281792	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





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Instrument : BNA_F
ClientSampleId : S2(0-5)

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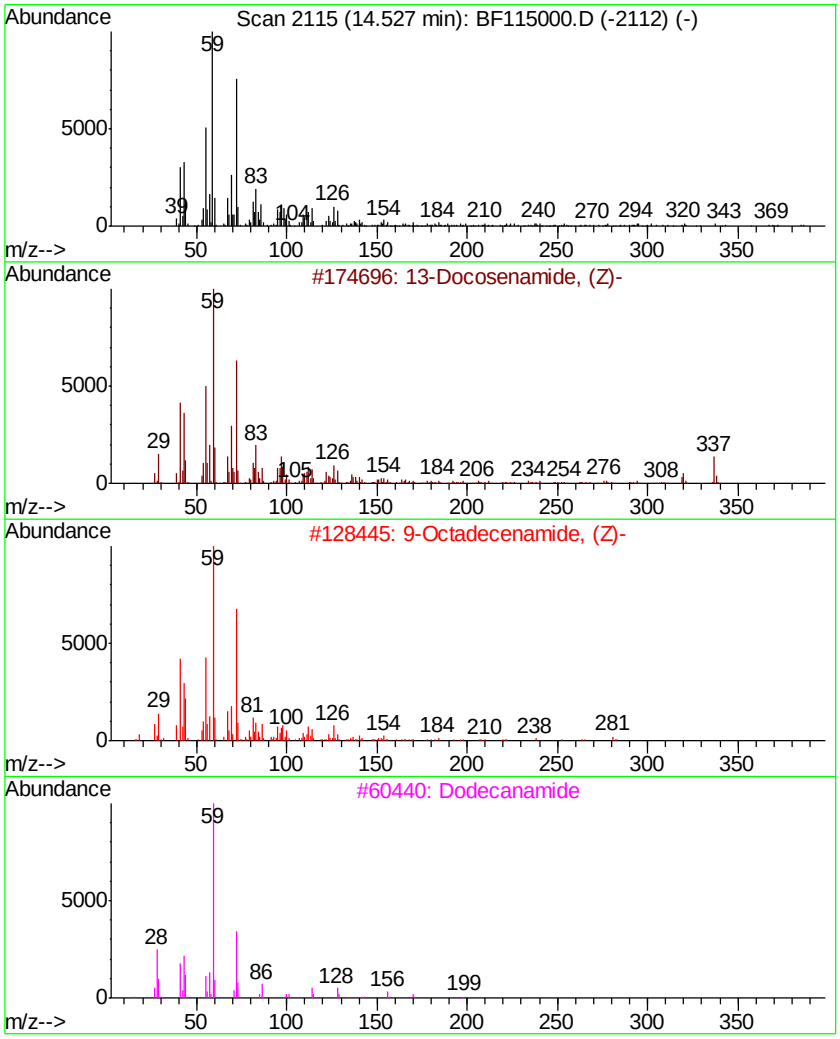
TIC Integration Parameters: LSCINT.P

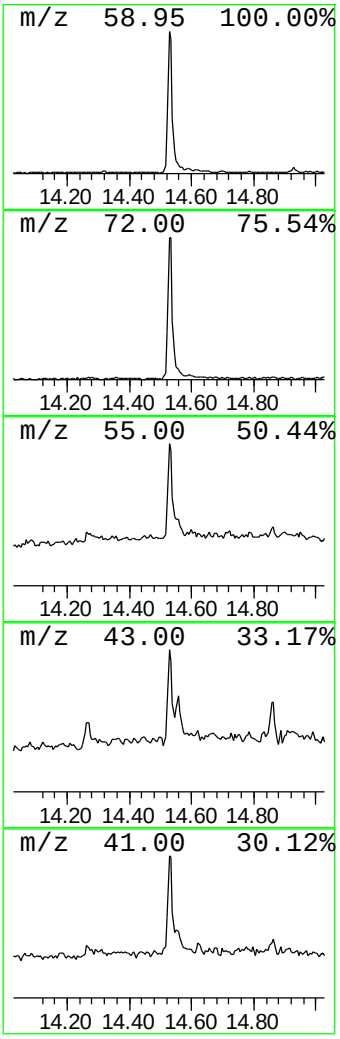
****

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	5.44 ng	364714	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Dodecanamide	199	C12H25NO	001120-16-7	50
4	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	43
5	Tetradecanamide	227	C14H29NO	000638-58-4	43





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

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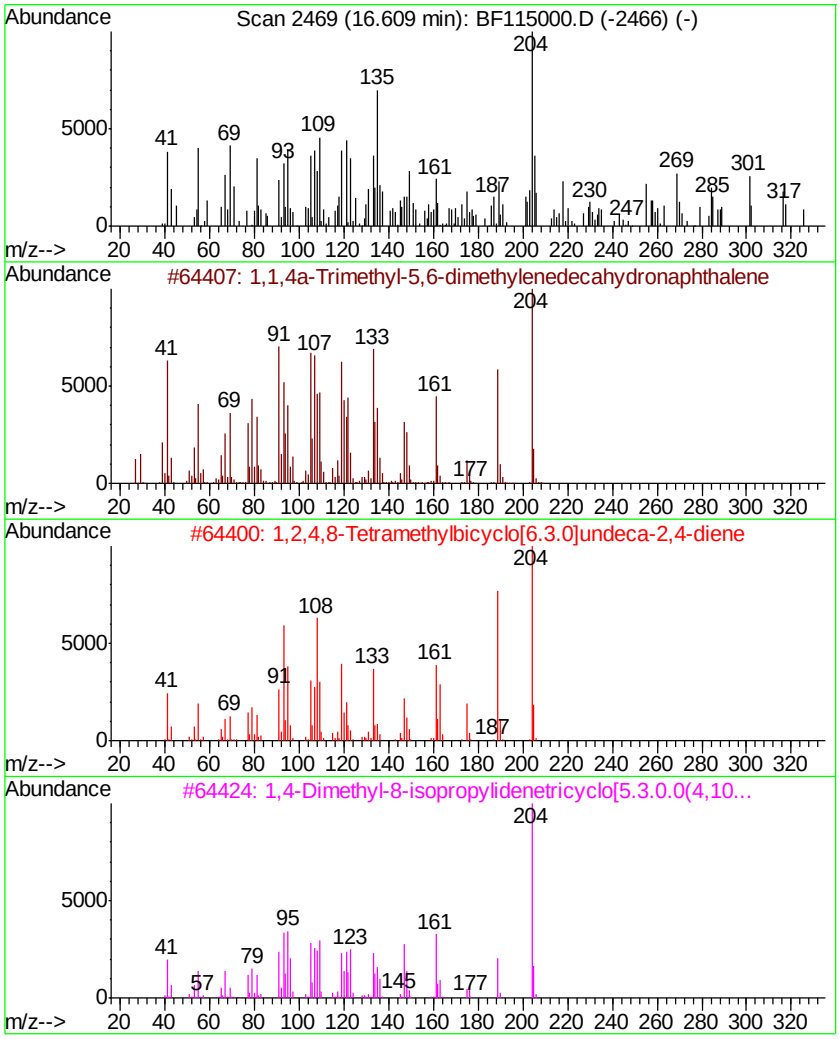
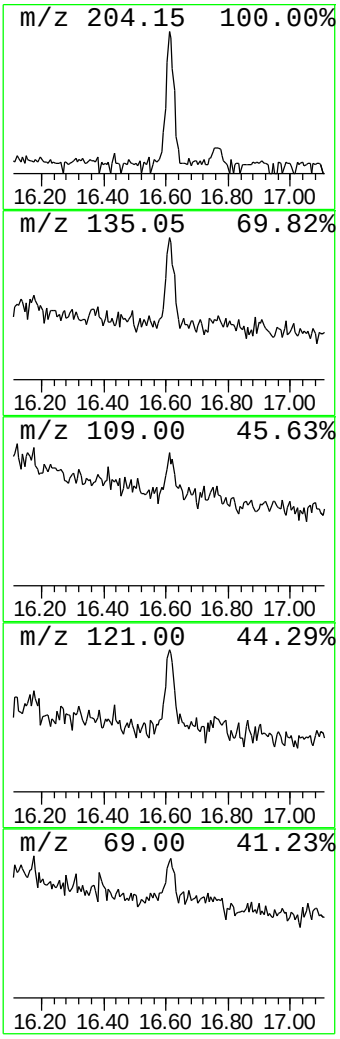
Peak Number 7 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	2.36 ng	157891	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	64
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	64
3	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	62
4	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	45
5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	38





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.18	68.3	ng	5332980	1	6.65	1561930	20.0
2-Pentanone, 4-hy...	4.86	102.1	ng	7971610	1	6.65	1561930	20.0
unknown6.41	6.41	13.4	ng	1049720	1	6.65	1561930	20.0
Behenic alcohol	13.64	3.9	ng	281792	5	13.77	1456820	20.0
13-Docosenamide, ...	14.53	5.4	ng	364714	6	15.14	1340690	20.0
1,1,4a-Trimethyl-...	16.61	2.4	ng	157891	6	15.14	1340690	20.0