LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112505.D
Acq On : 12 Feb 2019 11:54
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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-BF012519.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	5.045	500	503	516	rBV	61476	82687	4.25%	0.401%
2	5.469	572	575	593	rBV	1646029	1757260	90.25%	8.524%
3	6.487	744	748	765	rBV	1570573	1806212	92.77%	8.761%
4	6.610	765	769	776	rBV	2241199	1947058	100.00%	9.445%
5	6.834	803	807	815	rBV	709175	607234	31.19%	2.946%
6	6.987	830	833	841	rBV	1591042	1516124	77.87%	7.354%
7	7.398	899	903	913	rBV	1026784	1103975	56.70%	5.355%
8	8.116	1021	1025	1044	rVB	728185	718367	36.89%	3.485%
9	9.186	1203	1207	1218	rBV	2108824	1813539	93.14%	8.797%
10	9.580	1271	1274	1282	rVB	113112	120117	6.17%	0.583%
11	9.733	1296	1300	1306	rBV	62214	62770	3.22%	0.304%
12	9.869	1320	1323	1334	rVB	735587	710619	36.50%	3.447%
13	10.080	1352	1359	1363	rBV5	17621	23790	1.22%	0.115%
14	10.663	1454	1458	1468	rBV	1146977	1139823	58.54%	5.529%
15	10.780	1473	1478	1485	rVB5	31522	58108	2.98%	0.282%
16	10.969	1506	1510	1513	rBV5	17009	26186	1.34%	0.127%
17	11.210	1548	1551	1554	rBV	66102	61477	3.16%	0.298%
18	11.357	1573	1576	1579	rBV	734055	697973	35.85%	3.386%
19	11.380	1579	1580	1586	rVV	216685	187828	9.65%	0.911%
20	11.439	1587	1590	1593	rVV	58265	54249	2.79%	0.263%
21	11.598	1613	1617	1622	rBV3	29568	51537	2.65%	0.250%
22	11.639	1622	1624	1628	rVV3	26624	32022	1.64%	0.155%
23	11.704	1631	1635	1638	rBV5	20374	28398	1.46%	0.138%
24	11.880	1659	1665	1672	rBV3	273337	389969	20.03%	1.892%
25	11.939	1672	1675	1678	rVV	36293	42501	2.18%	0.206%
26	11.974	1678	1681	1683	rVV	87093	92281	4.74%	0.448%
27	11.998	1683	1685	1690	rVB	36278	31018	1.59%	0.150%
28	12.045	1690	1693	1696	rBV4	34351	30661	1.57%	0.149%
29	12.151	1709	1711	1715	rVB	33692	30493	1.57%	0.148%
30	12.198	1716	1719	1725	rVB7	26288	32842	1.69%	0.159%
31	12.410	1753	1755	1757	rBV	46425	37235	1.91%	0.181%
32	12.433	1757	1759	1763	rVV4	24689	30429	1.56%	0.148%
33	12.510	1769	1772	1774	rVB2	38860	37650	1.93%	0.183%
34	12.574	1780	1783	1788	rBV	758054	672392	34.53%	3.262%

LSC Area Percent Report

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Operator : JU/SJ
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.669	1796	1799	1802	rBV2	94542	122459	6.29%	0.594%
36	12.804	1816	1822	1829	rBV	709979	808625	41.53%	3.922%
37	12.939	1841	1845	1848	rBV	1946315	1624128	83.41%	7.878%
38	13.198	1887	1889	1892	rBV	52761	51299	2.63%	0.249%
39	13.833	1994	1997	2000	rBV3	195069	197306	10.13%	0.957%
40	14.004	2022	2026	2029	rBV2	854051	1091121	56.04%	5.293%
41	14.033	2029	2031	2035	rVB	312264	266618	13.69%	1.293%
42	14.451	2100	2102	2108	rBV2	141693	153679	7.89%	0.745%
43	15.057	2202	2205	2207	rBV	215181	265317	13.63%	1.287%

Sum of corrected areas: 20615376

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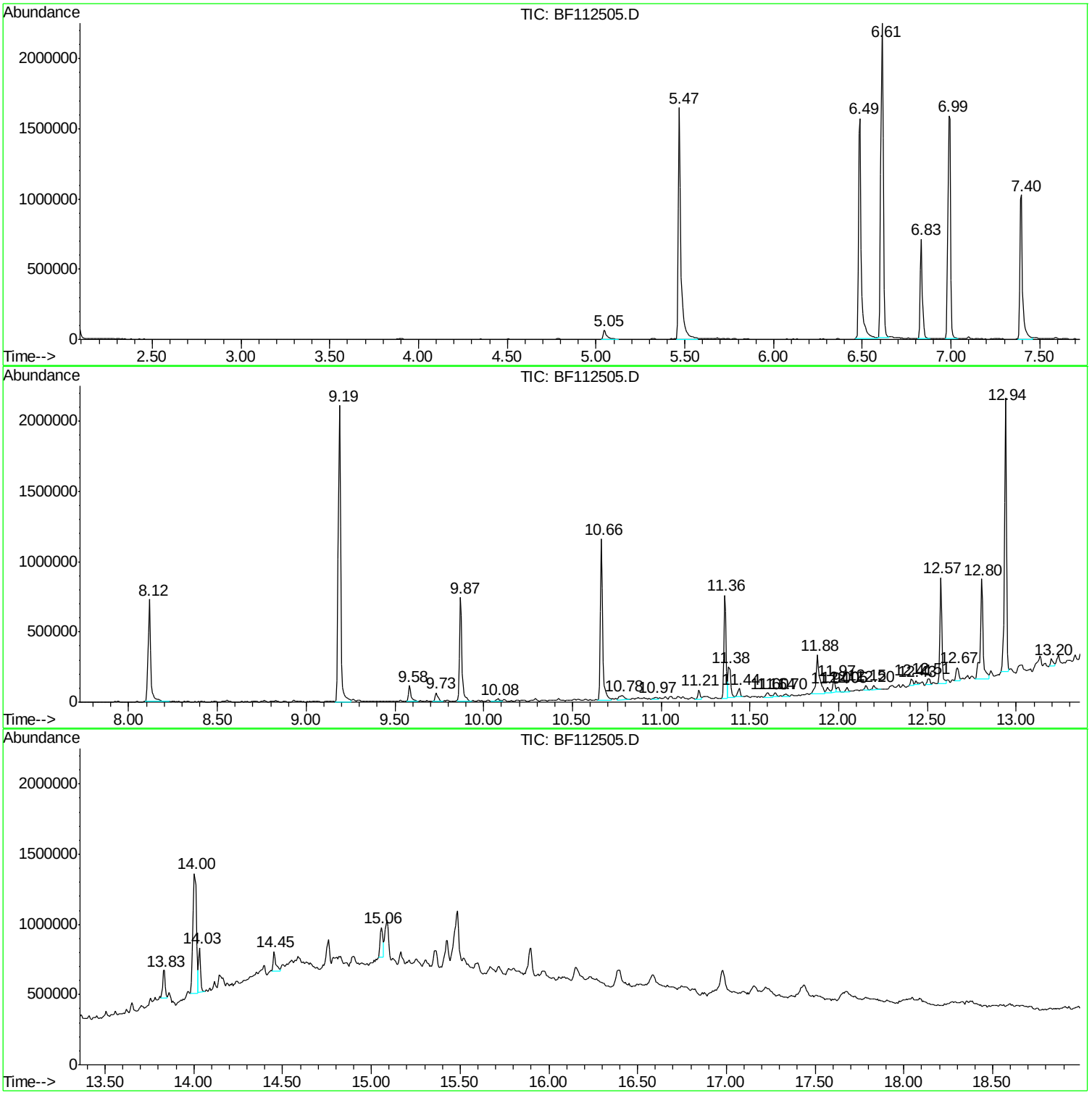
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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Data File : BF112505.D
Acq On : 12 Feb 2019 11:54
Operator : JU/SJ
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

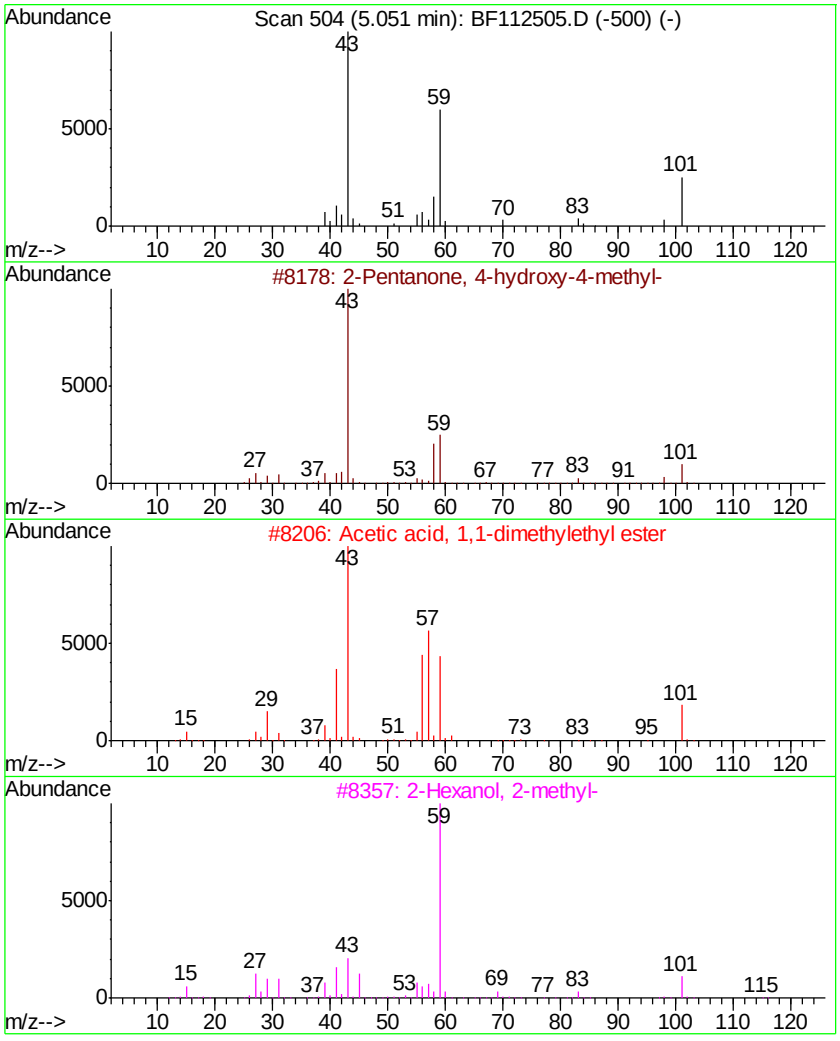
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

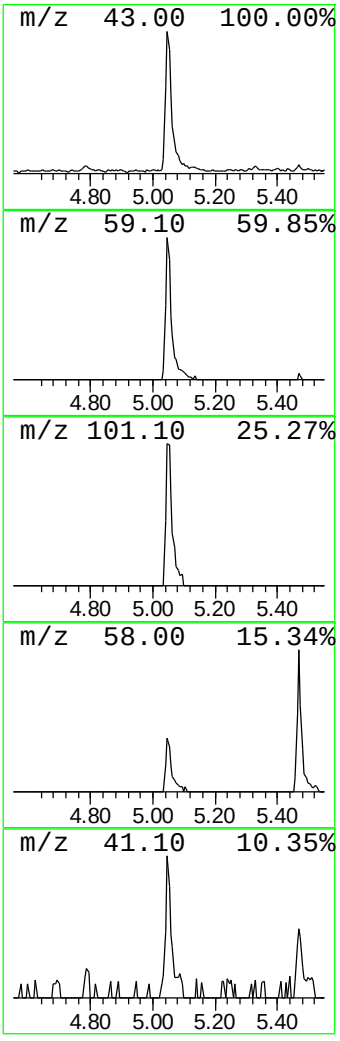
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	2.72 ng	82687	1,4-Dichlorobenzene-d4	6.83

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
4	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32





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Data File : BF112505.D
Acq On : 12 Feb 2019 11:54
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

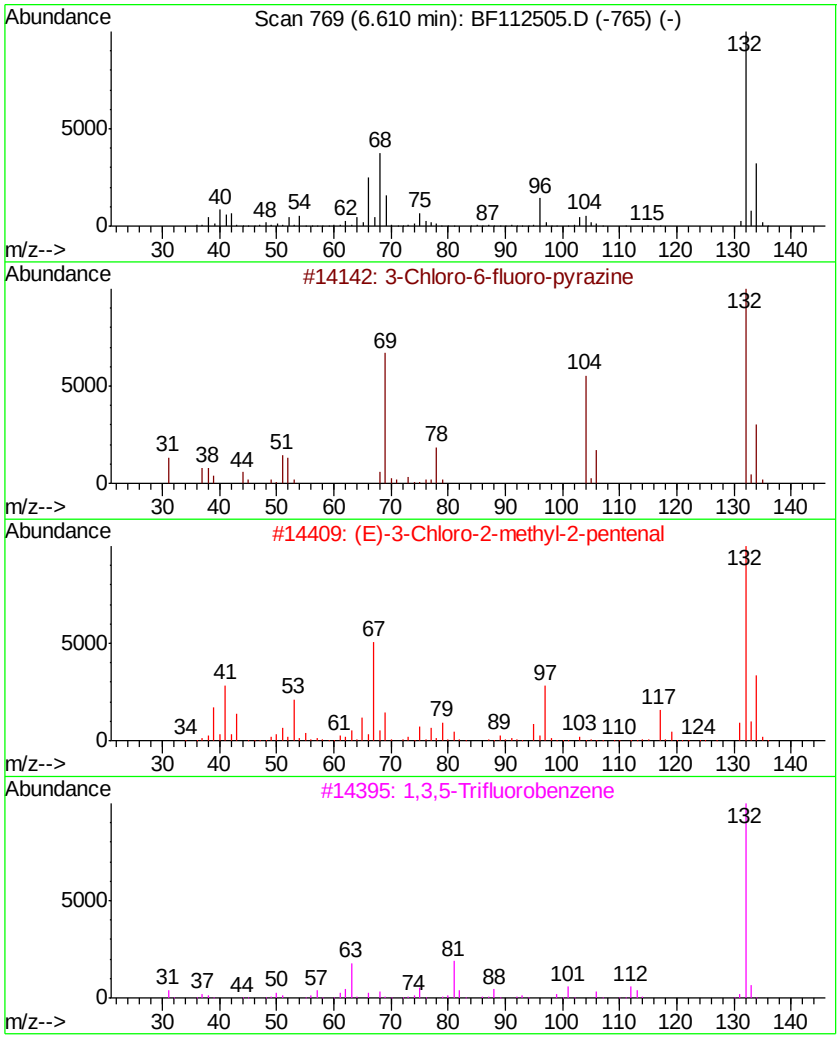
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

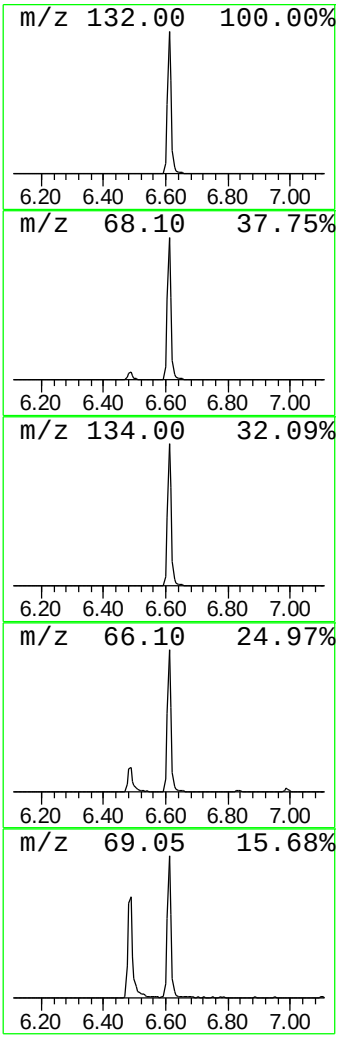
****

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	64.13 ng	1947060	1,4-Dichlorobenzene-d4	6.83

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	17
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
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Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

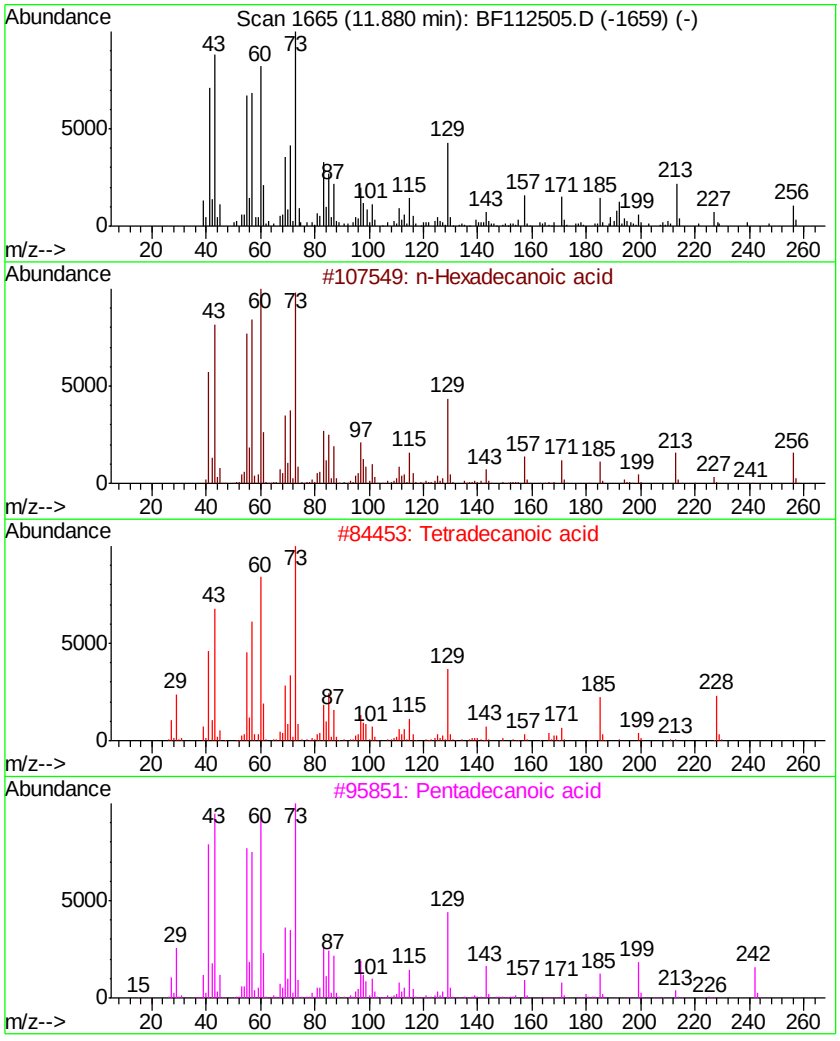
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

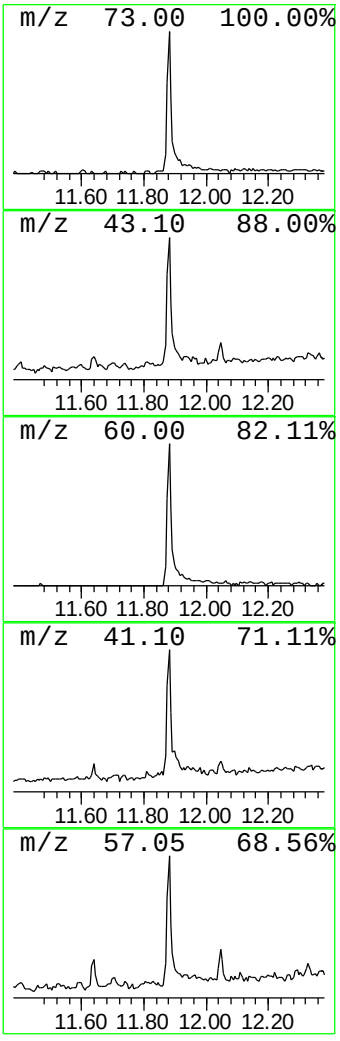
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	11.17 ng	389969	Phenanthrene-d10	11.36

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112505.D
Acq On : 12 Feb 2019 11:54
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

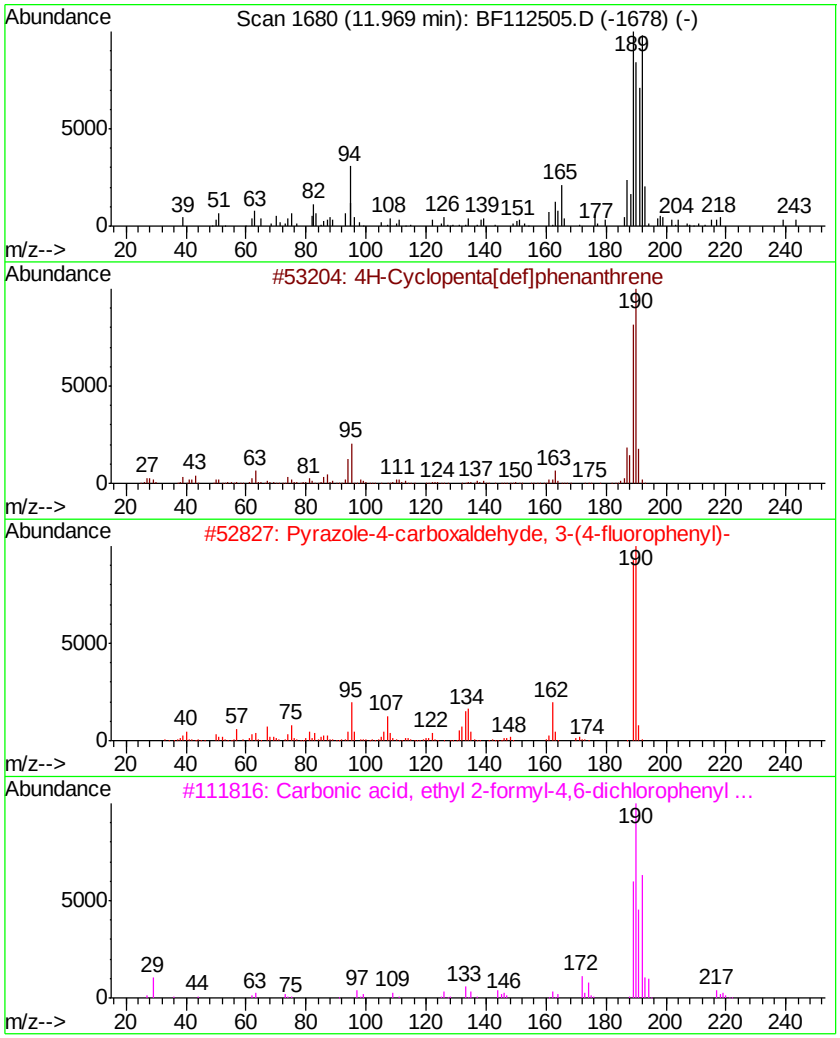
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

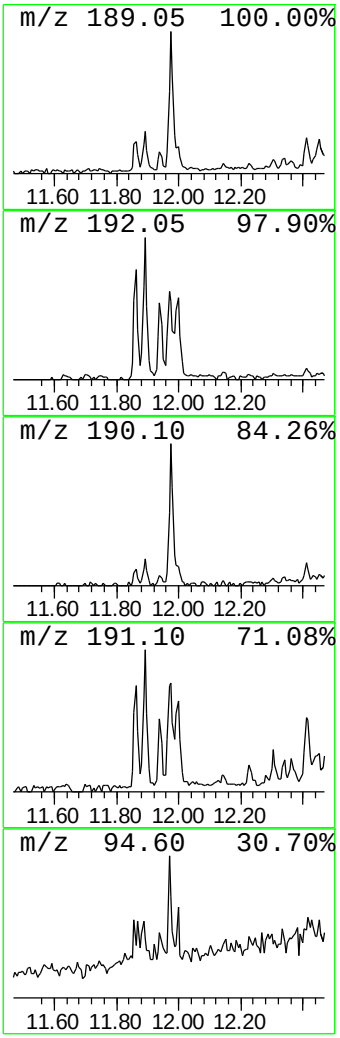
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	2.64 ng	92281	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	38
3	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	33
4	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	30
5	Carbonic acid, butyl 2-formyl-4,...	290	C12H12Cl2O4	1000331-42-2	25





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
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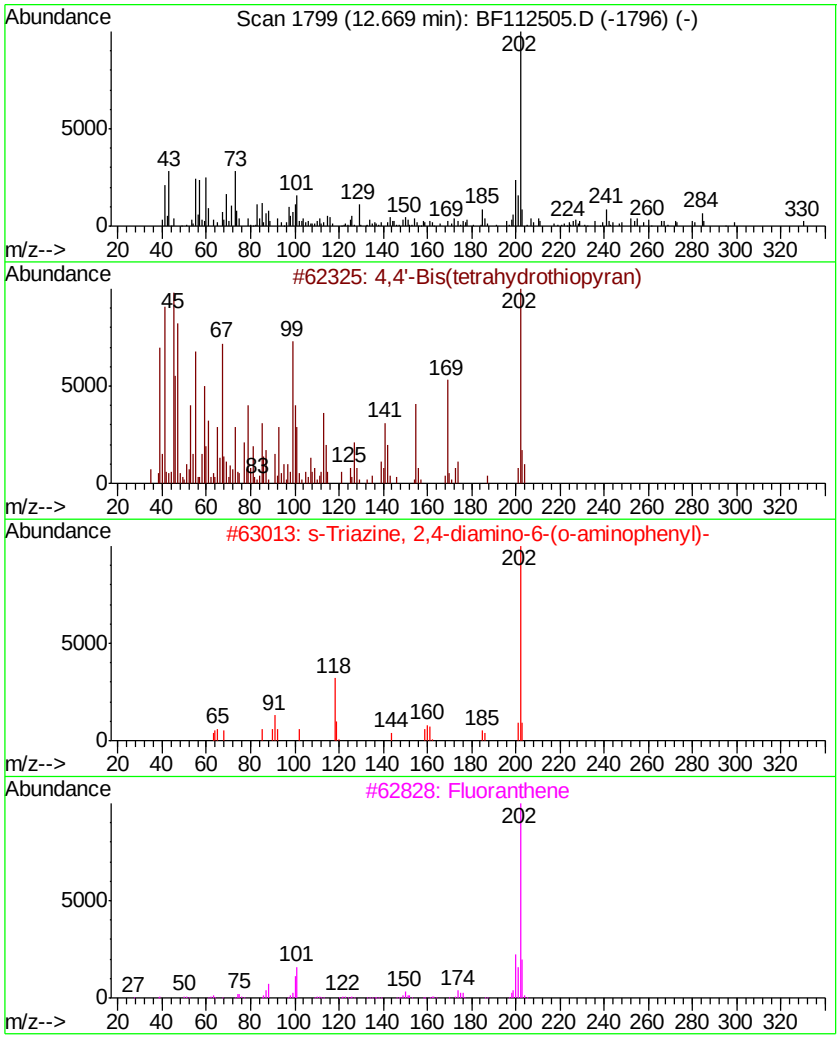
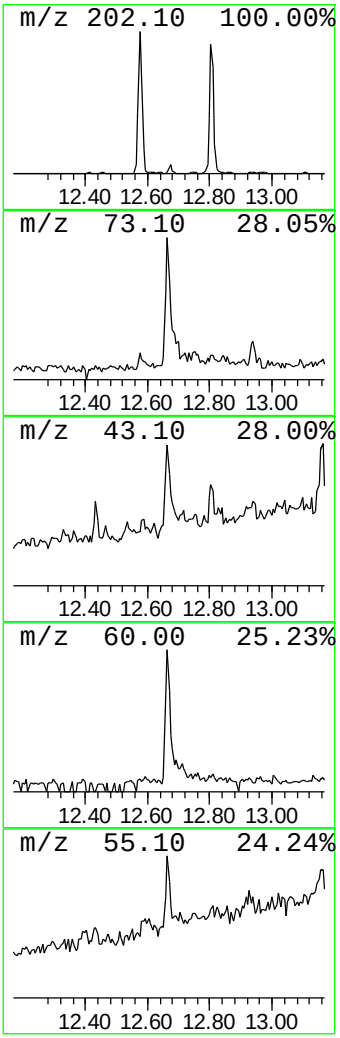
****

Peak Number 6 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	3.51 ng	122459	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	94
2	s-Triazine, 2,4-diamino-6-(o-ami...	202	C9H10N6	029366-74-3	47
3	Fluoranthene	202	C16H10	000206-44-0	45
4	Pyrene	202	C16H10	000129-00-0	43
5	Pyrimidine, 4-methoxy-6-(2-hydro...	202	C11H10N2O2	097630-79-0	38





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ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

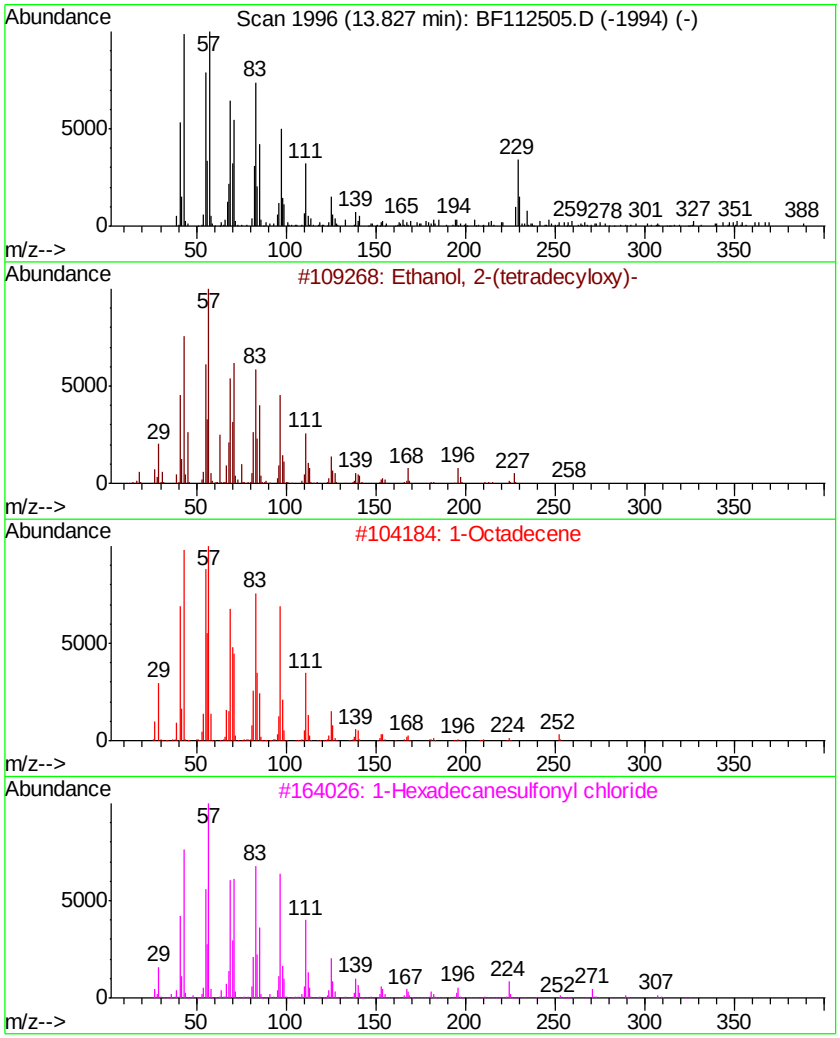
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

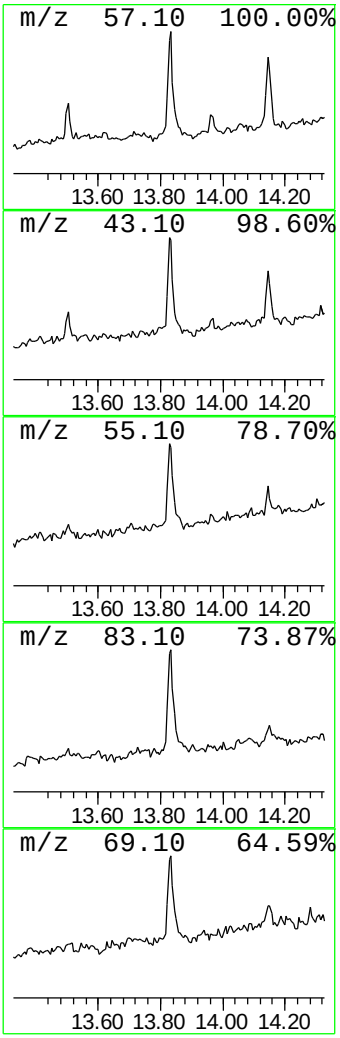
****

Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.62 ng	197306	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	94
2	1-Octadecene	252	C18H36	000112-88-9	91
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
4	Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	83
5	1-Nonadecene	266	C19H38	018435-45-5	78





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

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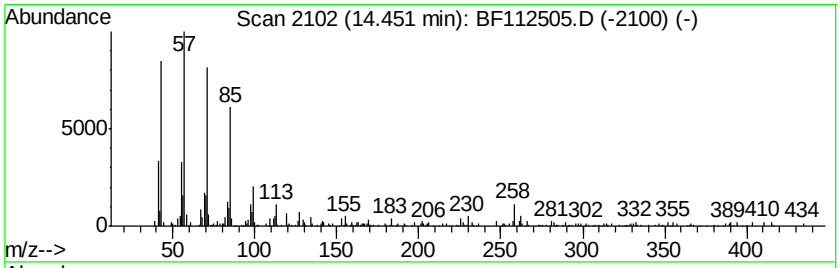
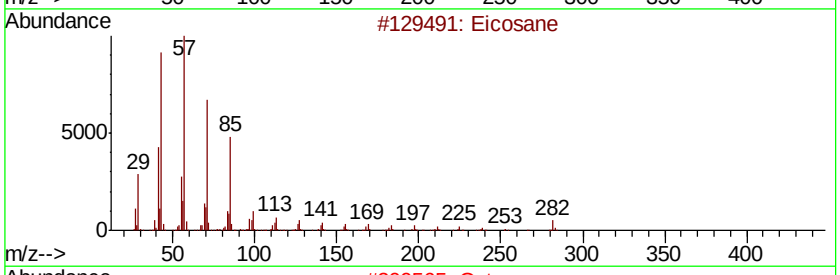
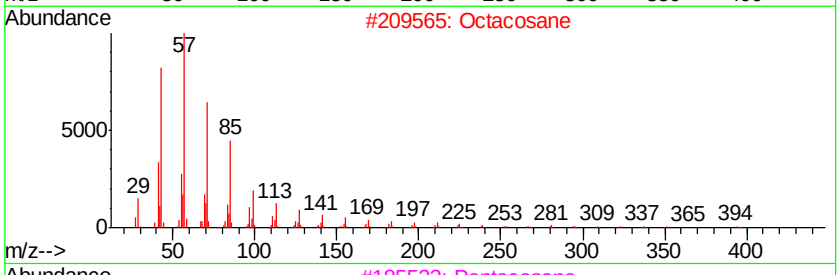
Peak Number 8 Eicosane Concentration Rank 6

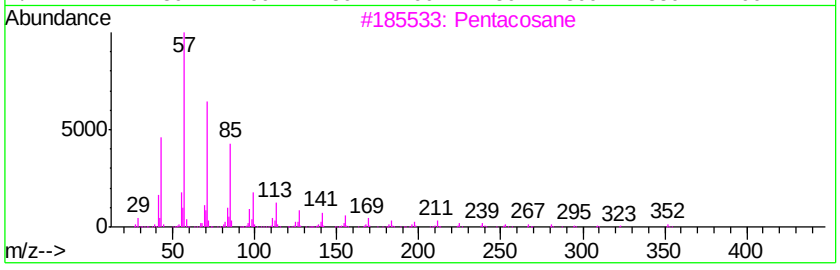
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.82 ng	153679	Chrysene-d12	14.01

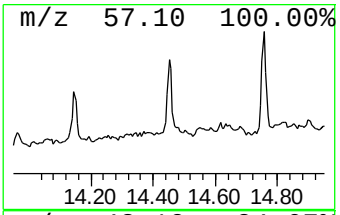
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octacosane	394	C28H58	000630-02-4	93
3	Pentacosane	352	C25H52	000629-99-2	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89
5	Hexacosane	366	C26H54	000630-01-3	74

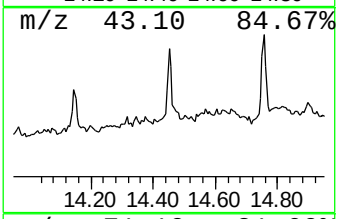


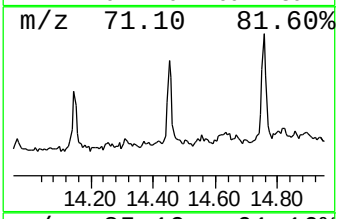


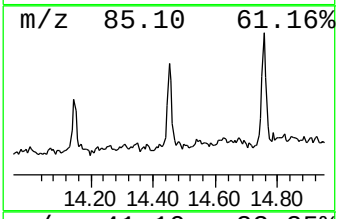


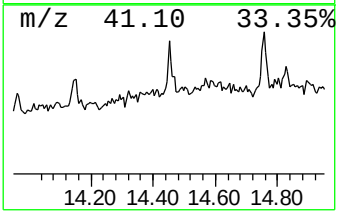












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021219\
Data File : BF112505.D
Acq On : 12 Feb 2019 11:54
Operator : JU/SJ
Sample : K1442-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
2-Pentanone, 4-hy...	5.05	2.7	ng	82687	1	6.83	607234	20.0
unknown6.61	6.61	64.1	ng	1947060	1	6.83	607234	20.0
n-Hexadecanoic acid	11.88	11.2	ng	389969	4	11.36	697973	20.0
4H-Cyclopenta[def...	11.97	2.6	ng	92281	4	11.36	697973	20.0
4,4'-Bis(tetrahyd...	12.67	3.5	ng	122459	4	11.36	697973	20.0
Ethanol, 2-(tetra...	13.83	3.6	ng	197306	5	14.01	1091120	20.0
Eicosane	14.45	2.8	ng	153679	5	14.01	1091120	20.0