LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116897.D
Acq On : 9 Sep 2019 15:31
Operator : HP/JU
Sample : PB122916BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122916BL

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-BF083019.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	2.169	7	14	23	rVB	66845	97521	2.68%	0.346%
2	5.469	569	575	578	rBV	2676862	2903287	79.64%	10.305%
3	6.475	740	746	749	rBV	2484956	3100411	85.05%	11.005%
4	6.610	764	769	772	rBV	3119782	3163443	86.77%	11.229%
5	6.834	804	807	811	rBV	678652	571804	15.68%	2.030%
6	6.992	830	834	838	rBV	2505042	2424740	66.51%	8.607%
7	7.398	897	903	906	rBV	1818936	1913201	52.48%	6.791%
8	8.116	1020	1025	1044	rBV	730497	732935	20.10%	2.602%
9	9.192	1202	1208	1211	rBV	3864694	3645587	100.00%	12.940%
10	9.869	1318	1323	1337	rBV	880873	833306	22.86%	2.958%
11	10.657	1452	1457	1478	rBV	2071755	2142088	58.76%	7.603%
12	11.351	1571	1575	1583	rBV	816039	799949	21.94%	2.839%
13	12.939	1839	1845	1848	rBV	3352475	3581206	98.23%	12.712%
14	13.986	2018	2023	2032	rVB	682651	699115	19.18%	2.482%
15	14.445	2096	2101	2104	rBV3	53380	57030	1.56%	0.202%
16	14.751	2148	2153	2157	rBV	98575	107107	2.94%	0.380%
17	15.080	2204	2209	2215	rVB	151354	174298	4.78%	0.619%
18	15.439	2264	2270	2279	rBV2	456135	818475	22.45%	2.905%
19	15.880	2338	2345	2356	rVB2	143853	223524	6.13%	0.793%
20	16.380	2423	2430	2437	rBV	73953	128897	3.54%	0.458%
21	16.956	2522	2528	2535	rVB2	26399	54527	1.50%	0.194%

Sum of corrected areas: 28172451

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116897.D
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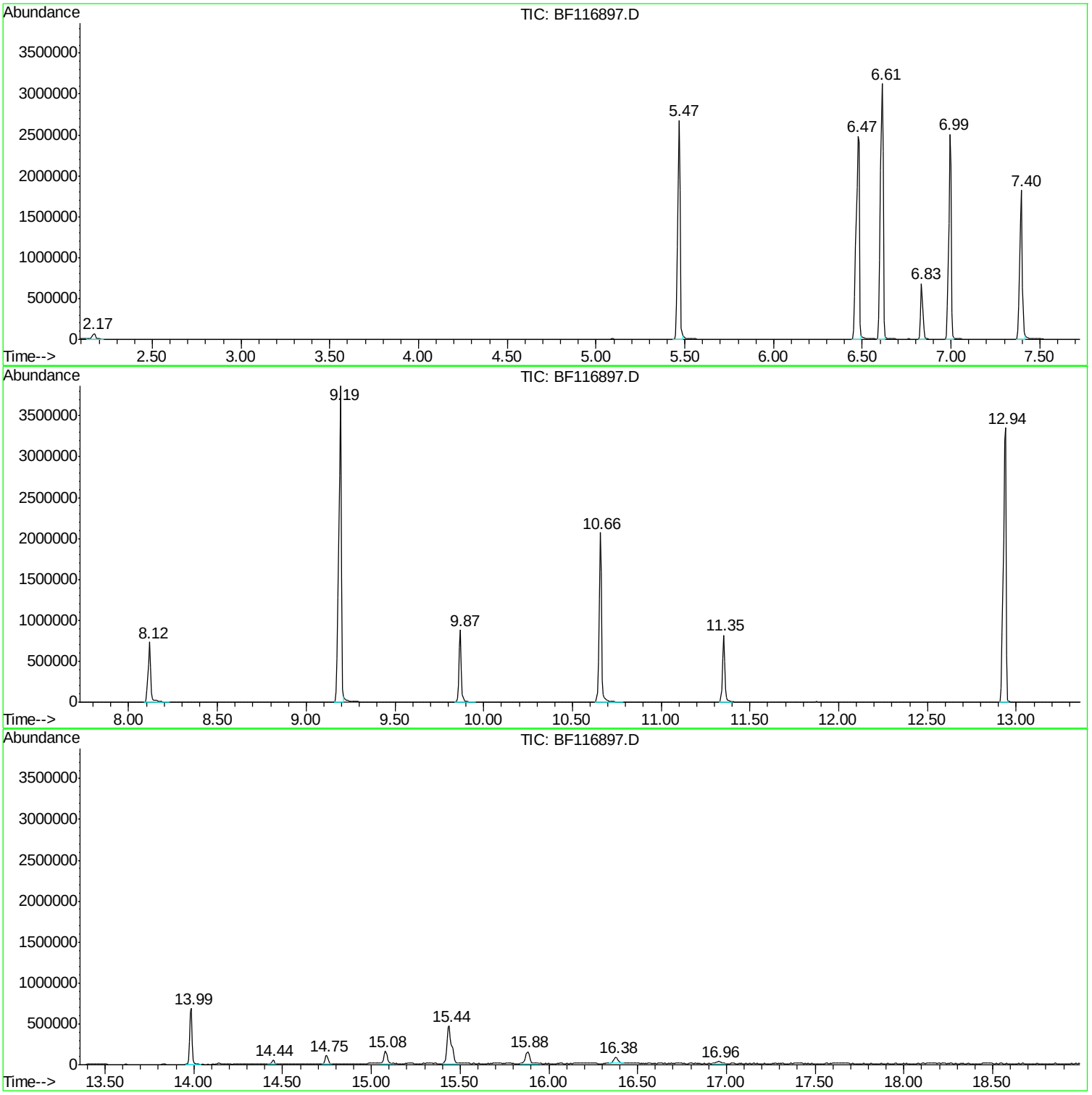
Operator : HP/JU
Sample : PB122916BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122916BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116897.D
Acq On : 9 Sep 2019 15:31
Operator : HP/JU
Sample : PB122916BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB122916BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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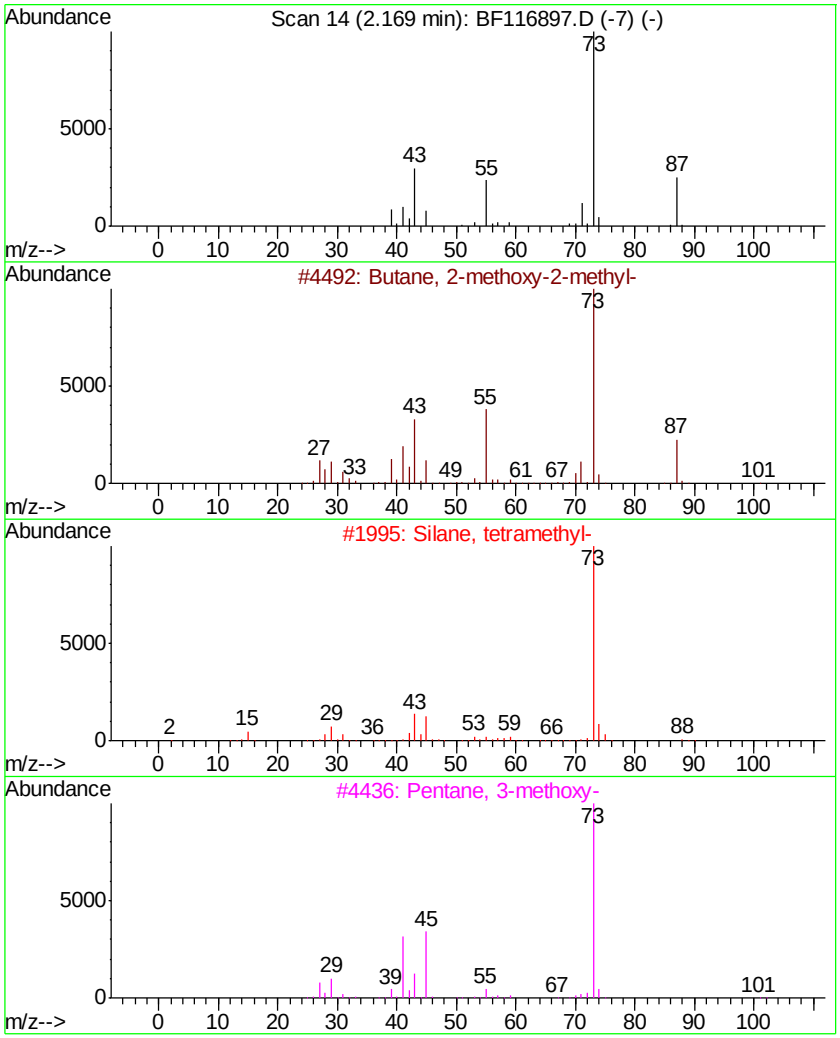
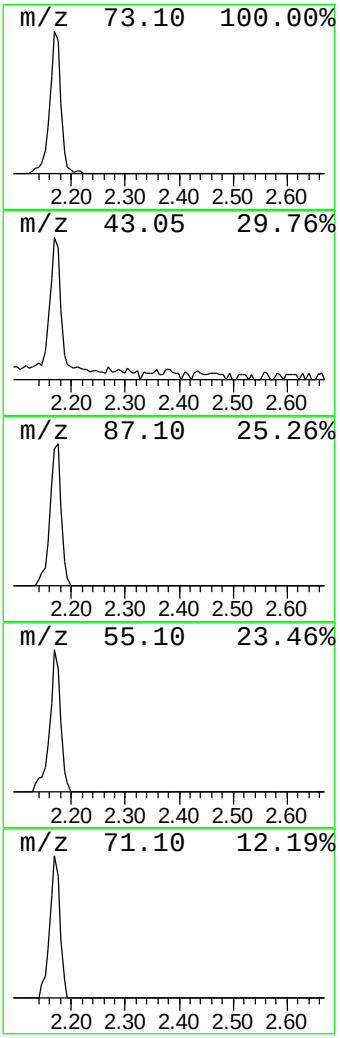
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	3.41 ng	97521	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116897.D
Acq On : 9 Sep 2019 15:31
Operator : HP/JU
Sample : PB122916BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122916BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

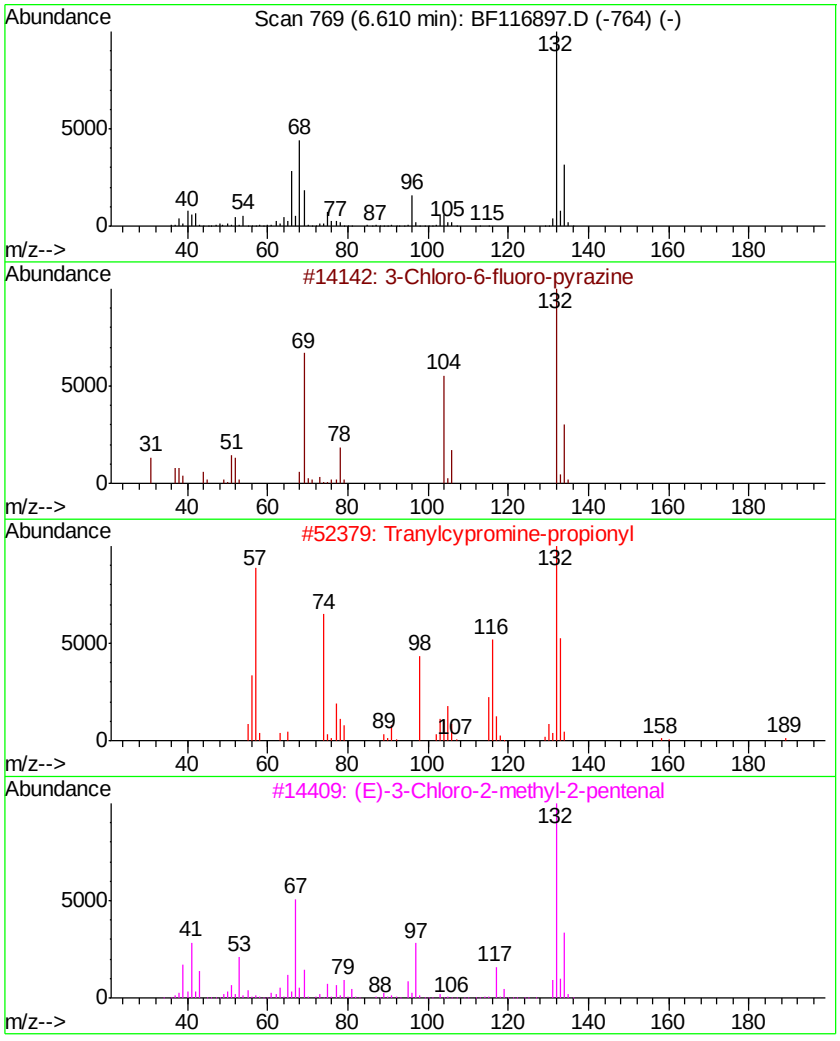
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

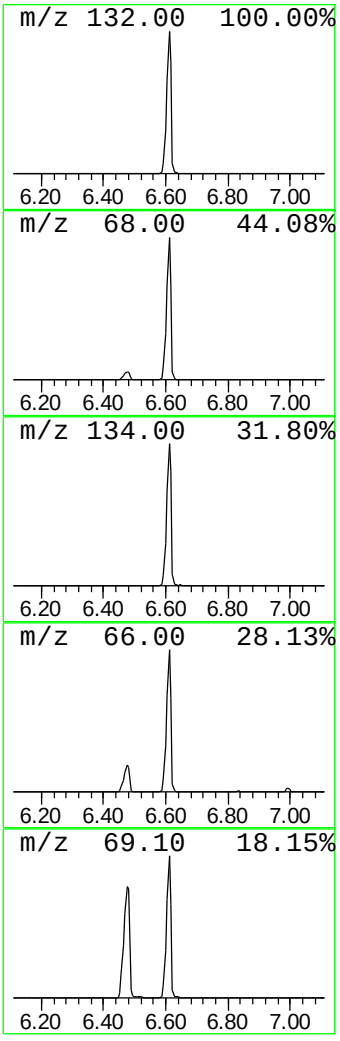
****

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	110.65 ng	3163440	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	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116897.D
Acq On : 9 Sep 2019 15:31
Operator : HP/JU
Sample : PB122916BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122916BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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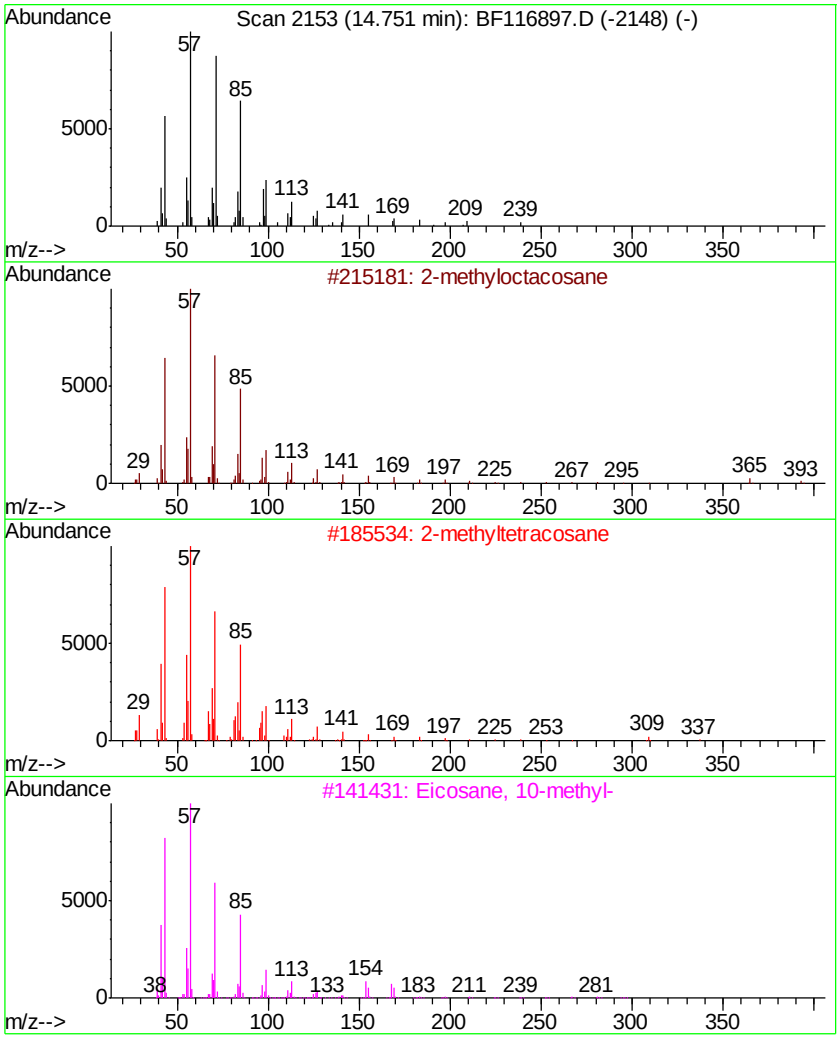
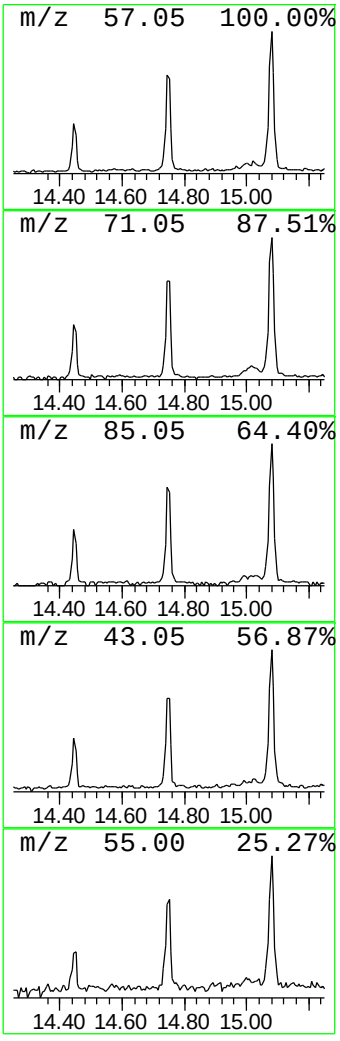
Peak Number 4 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.62 ng	107107	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	2-methyltetracosane	352	C25H52	1000376-72-6	90
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Hexacosane	366	C26H54	000630-01-3	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090919\
Data File : BF116897.D
Acq On : 9 Sep 2019 15:31
Operator : HP/JU
Sample : PB122916BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122916BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

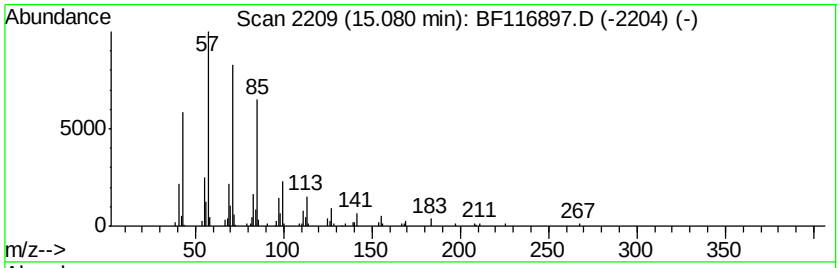
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

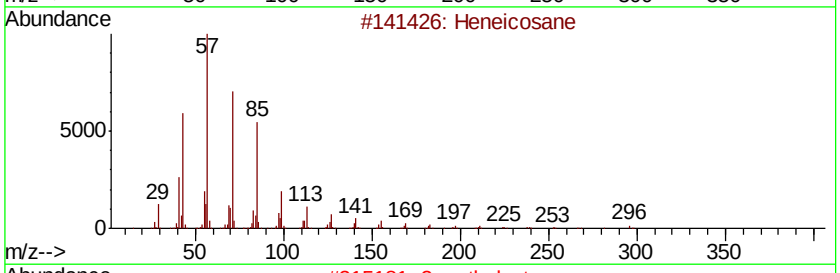
****

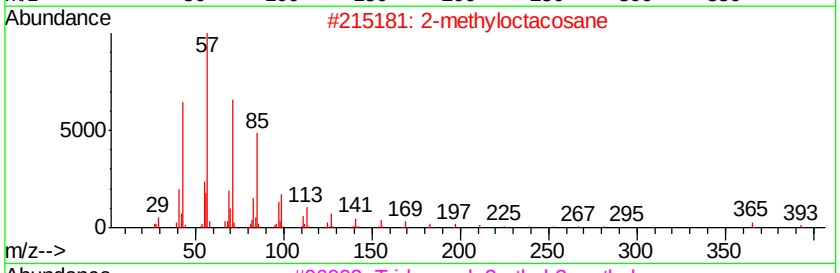
Peak Number 5 Heneicosane Concentration Rank 4

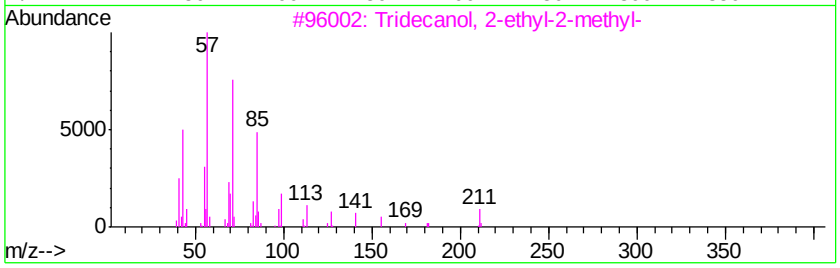
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	4.26 ng	174298	Perylene-d12	15.43

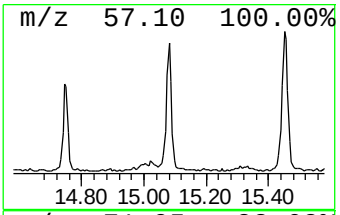
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86

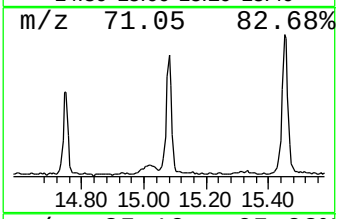


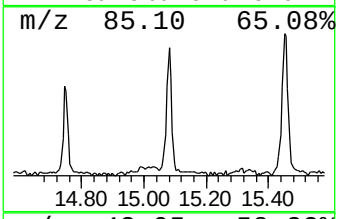


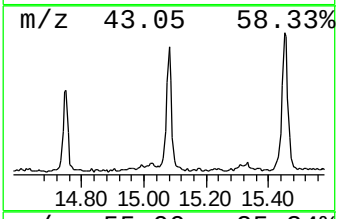


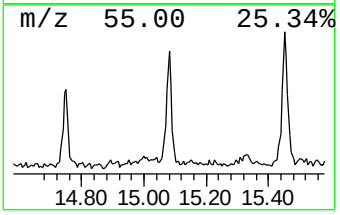












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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

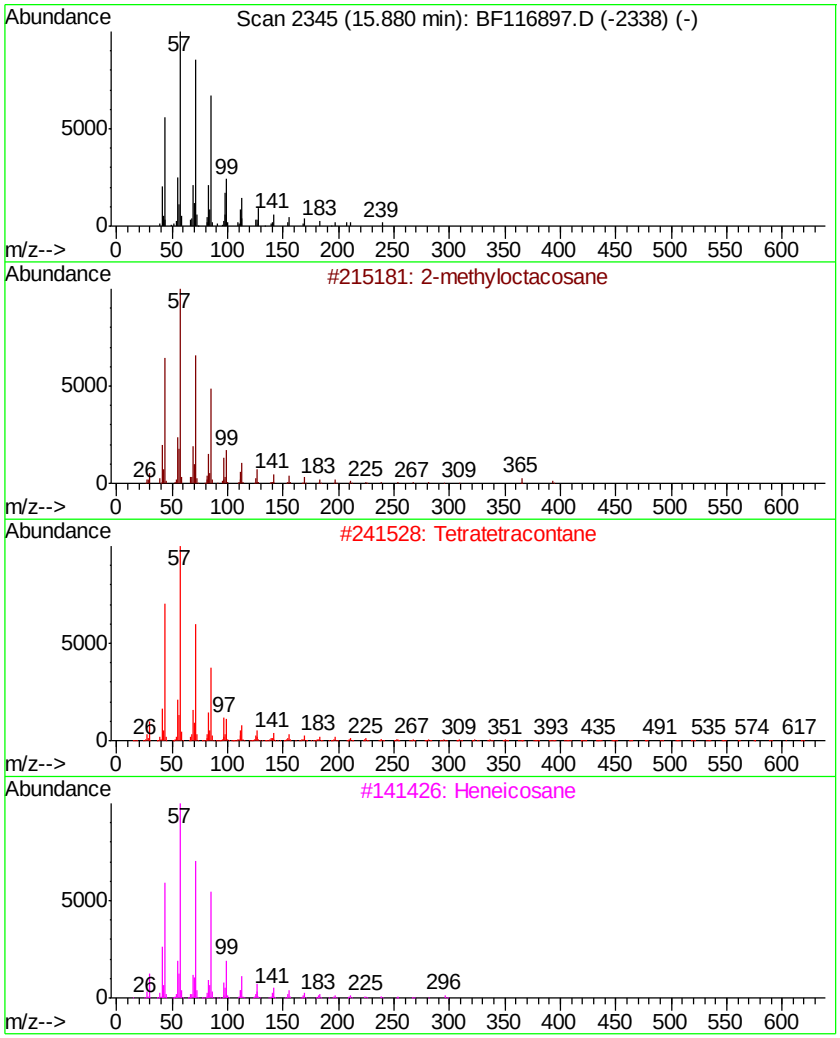
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

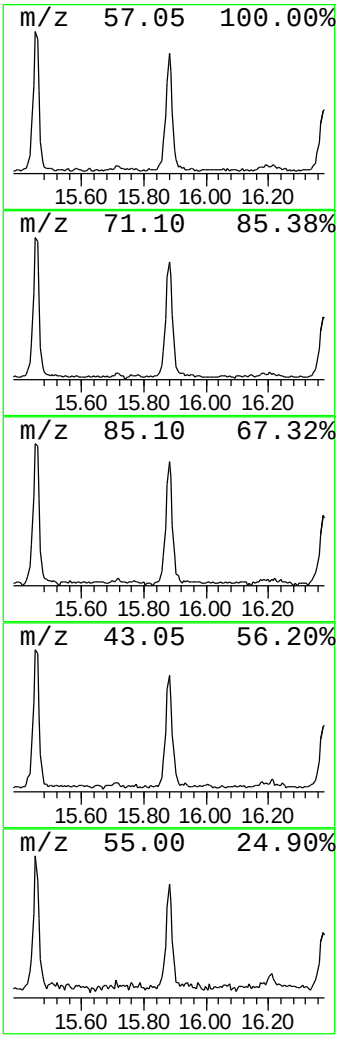
****

Peak Number 6 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	5.46 ng	223524	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Heneicosane	296	C21H44	000629-94-7	83
4	Hexacosane	366	C26H54	000630-01-3	83
5	Tritetracontane	605	C43H88	007098-21-7	80





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Sample : PB122916BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB122916BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

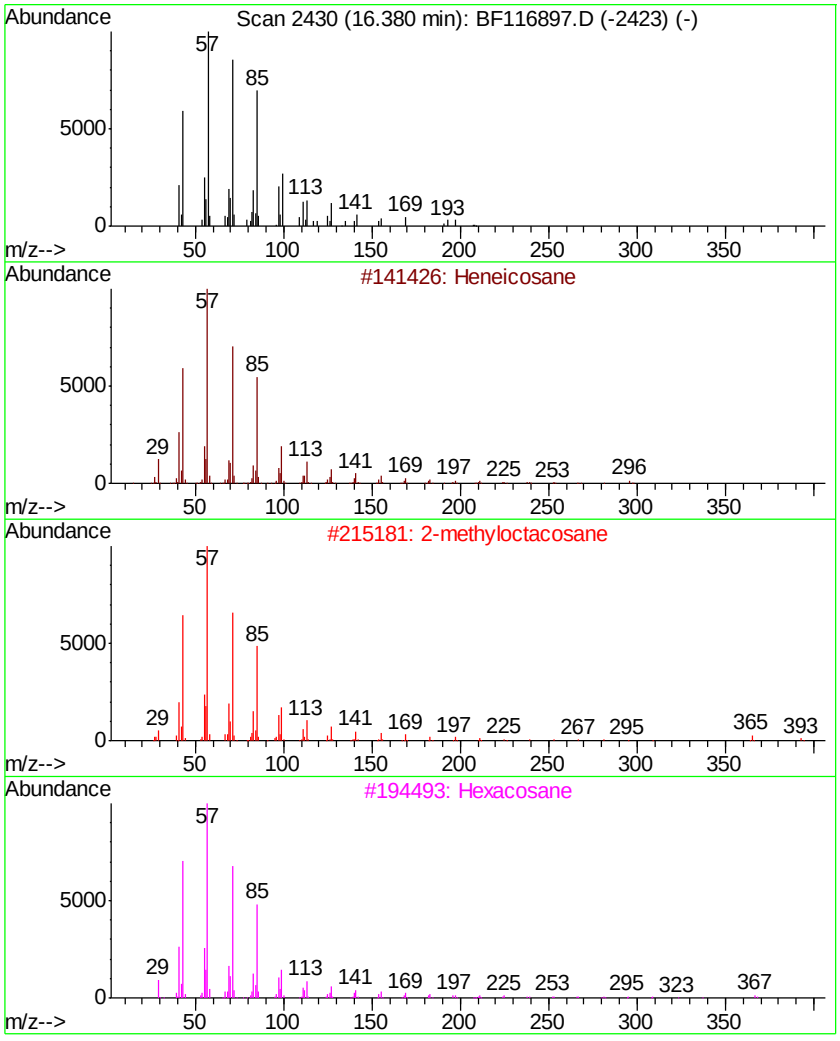
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

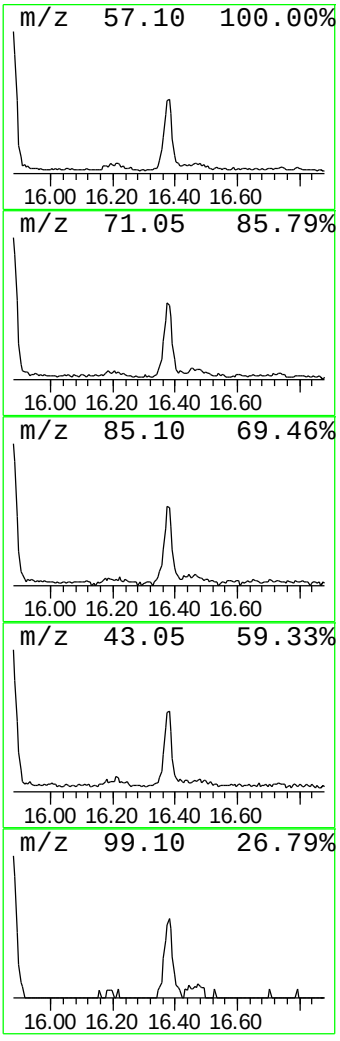
****

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	3.15 ng	128897	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	80
2	2-methyloctacosane	408	C29H60	1000376-72-8	80
3	Hexacosane	366	C26H54	000630-01-3	80
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5	Heptacosane	380	C27H56	000593-49-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090919\
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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
Butane, 2-methoxy...	2.17	3.4	ng	97521	1	6.83	571804	20.0
unknown6.61	6.61	110.7	ng	3163440	1	6.83	571804	20.0
2-methyloctacosane	14.75	2.6	ng	107107	6	15.43	818475	20.0
Heneicosane	15.08	4.3	ng	174298	6	15.43	818475	20.0
Tetratetracontane	15.88	5.5	ng	223524	6	15.43	818475	20.0
Hexacosane	16.38	3.1	ng	128897	6	15.43	818475	20.0