LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

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-BF051019.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	2.128	3	7	22	rVB	1419231	1950491	29.05%	3.155%
2	5.081	506	509	522	rVB	44827	73320	1.09%	0.119%
3	5.475	571	576	600	rBV	5646942	6154913	91.66%	9.955%
4	6.487	742	748	758	rBV	5634208	6542139	97.43%	10.581%
5	6.616	765	770	773	rBV	6005611	6114943	91.07%	9.890%
6	6.834	804	807	815	rBV	1579025	1390923	20.71%	2.250%
7	6.992	830	834	847	rBV	5253146	4852927	72.27%	7.849%
8	7.398	898	903	916	rBV	3973964	4191226	62.42%	6.779%
9	8.116	1021	1025	1046	rVB	1836069	1770972	26.37%	2.864%
10	8.581	1101	1104	1123	rBV	474330	946213	14.09%	1.530%
11	9.186	1202	1207	1218	rBV	6585898	6714690	100.00%	10.860%
12	9.580	1270	1274	1283	rBV	718027	678841	10.11%	1.098%
13	9.869	1319	1323	1333	rVB	2073870	1955260	29.12%	3.162%
14	10.657	1453	1457	1469	rBV	3889377	4116967	61.31%	6.659%
15	11.351	1571	1575	1585	rBV	2127443	2138528	31.85%	3.459%
16	11.874	1660	1664	1674	rBV	203281	285835	4.26%	0.462%
17	12.568	1779	1782	1789	rBV	159156	169678	2.53%	0.274%
18	12.657	1794	1797	1804	rBV2	51471	82063	1.22%	0.133%
19	12.798	1816	1821	1824	rBV	148550	158783	2.36%	0.257%
20	12.933	1839	1844	1848	rBV	5842830	6372559	94.90%	10.307%
21	13.827	1989	1996	2007	rBV2	243229	453866	6.76%	0.734%
22	13.992	2020	2024	2033	rVB	1741652	1826418	27.20%	2.954%
23	14.145	2046	2050	2053	rBV	93685	98735	1.47%	0.160%
24	14.451	2099	2102	2106	rBV2	124902	130657	1.95%	0.211%
25	14.757	2151	2154	2158	rVB	155895	154081	2.29%	0.249%
26	15.051	2200	2204	2207	rBV	66624	103604	1.54%	0.168%
27	15.092	2207	2211	2216	rVB2	169168	200130	2.98%	0.324%
28	15.468	2270	2275	2286	rBV	1300244	1704515	25.38%	2.757%
29	15.892	2343	2347	2353	rVB	155318	214498	3.19%	0.347%
30	16.392	2427	2432	2439	rVB	101491	172621	2.57%	0.279%
31	16.968	2525	2530	2538	rVB5	49561	108944	1.62%	0.176%

Sum of corrected areas: 61829340

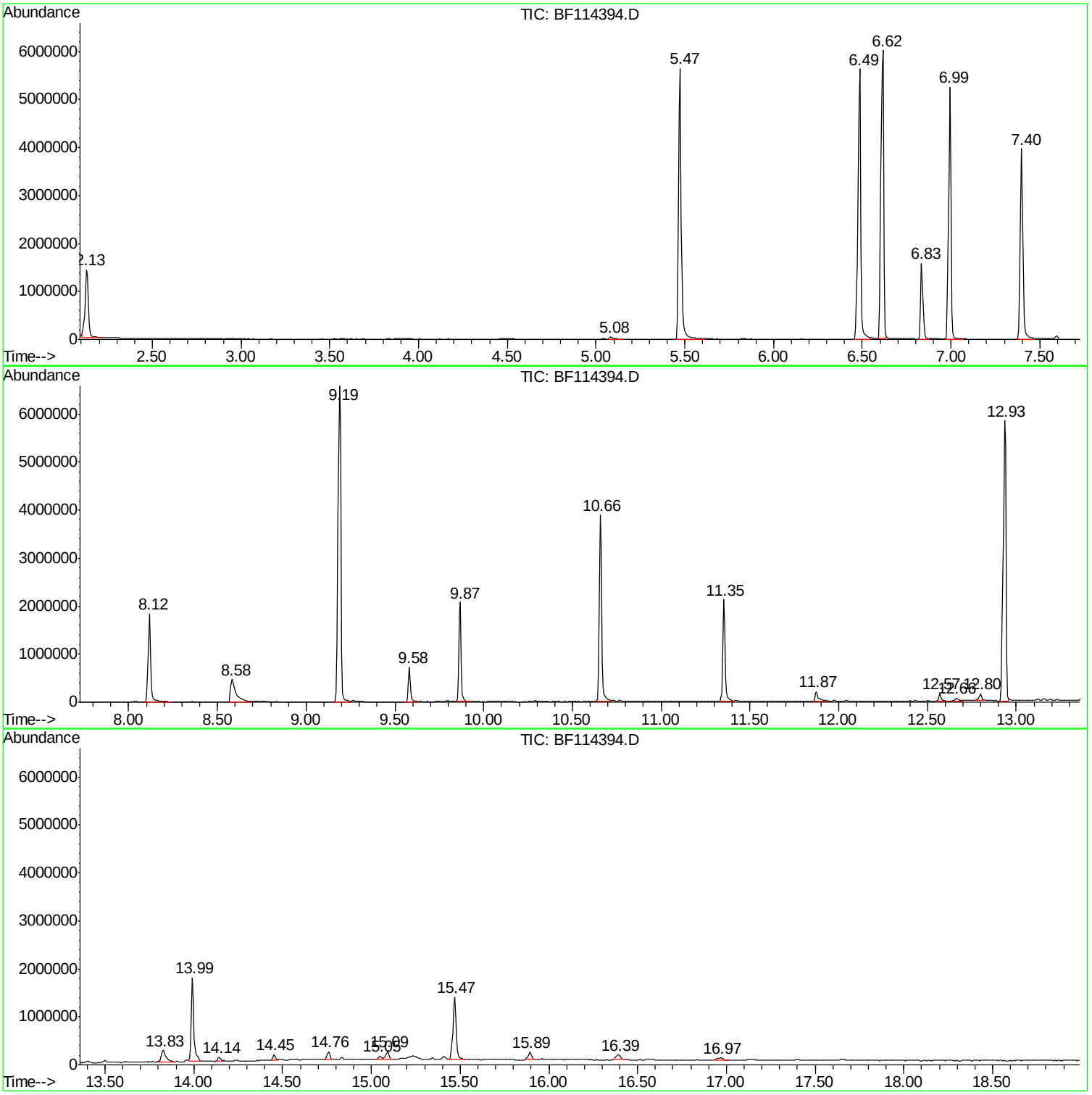
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF051819\
Data File : BF114394.D
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Instrument : BNA_F
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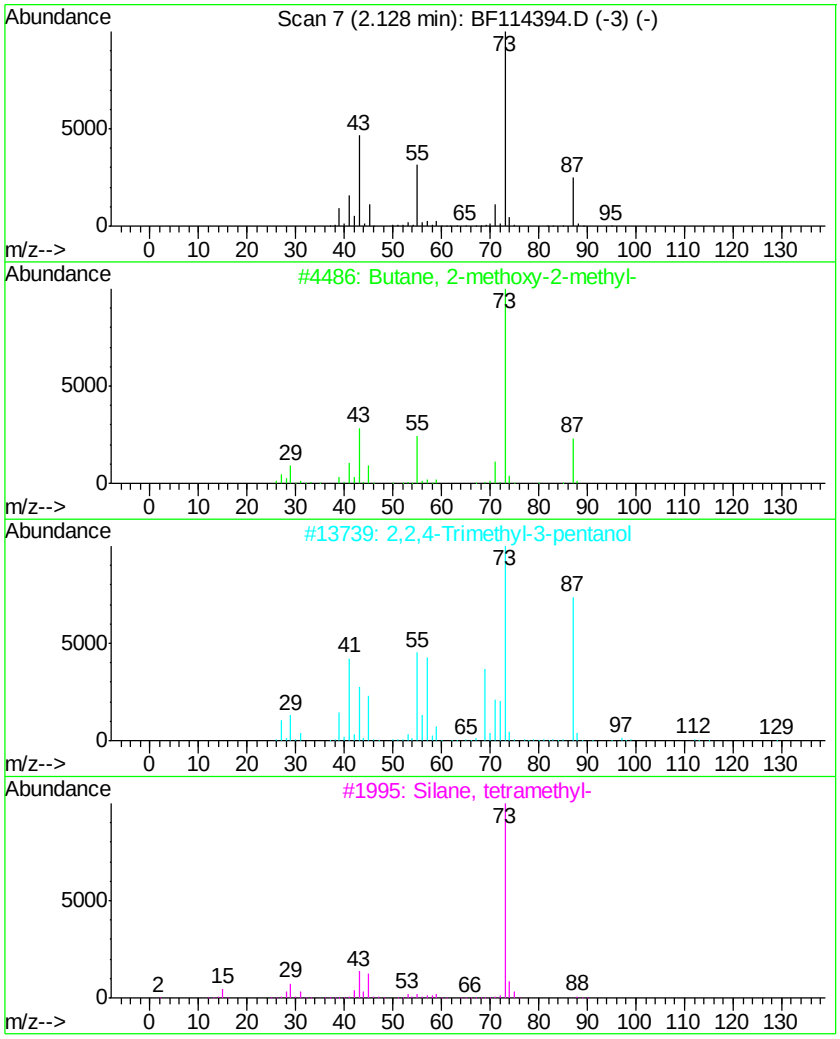
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

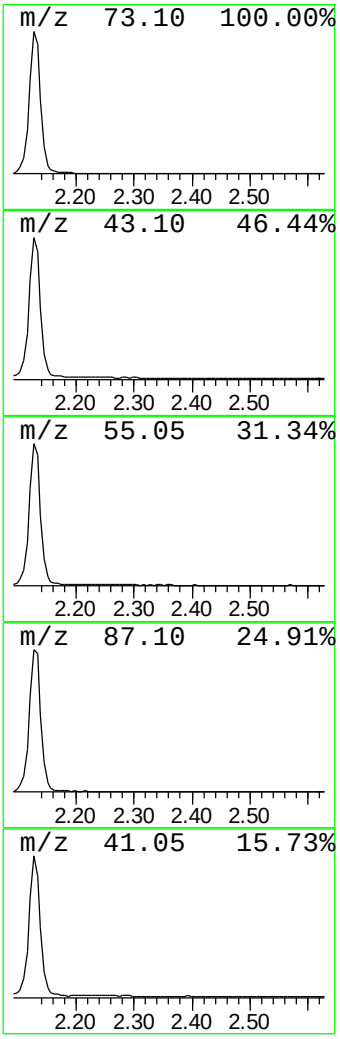
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	28.05 ng	1950490	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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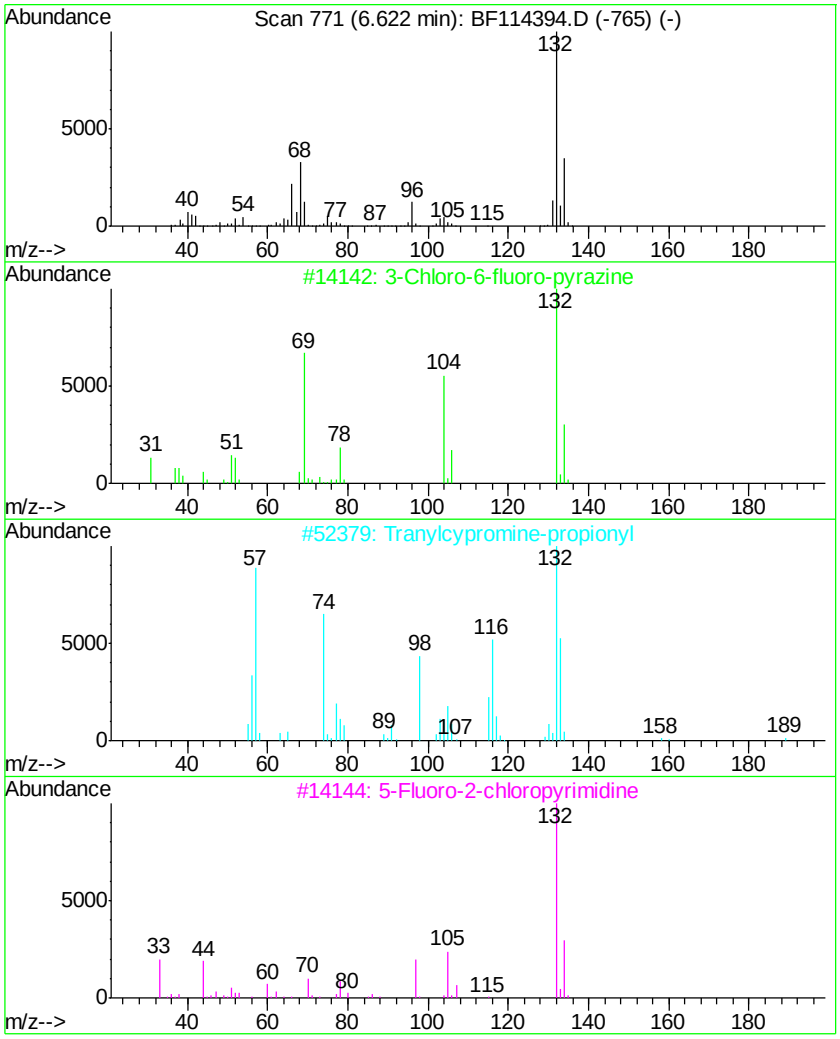
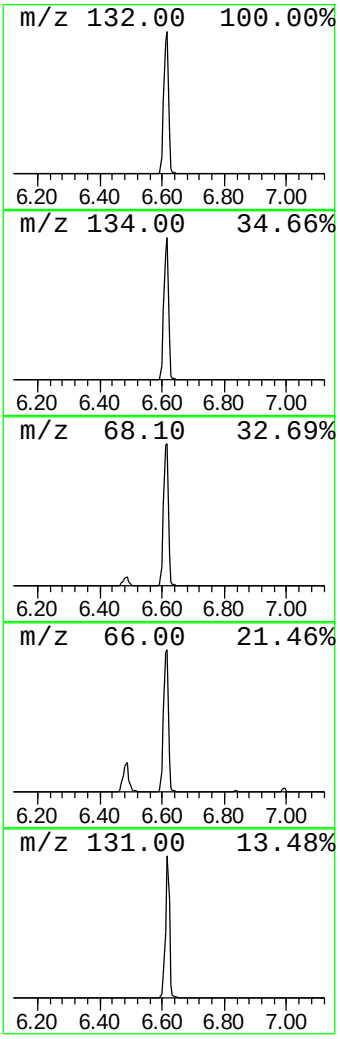
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	87.93 ng	6114940	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	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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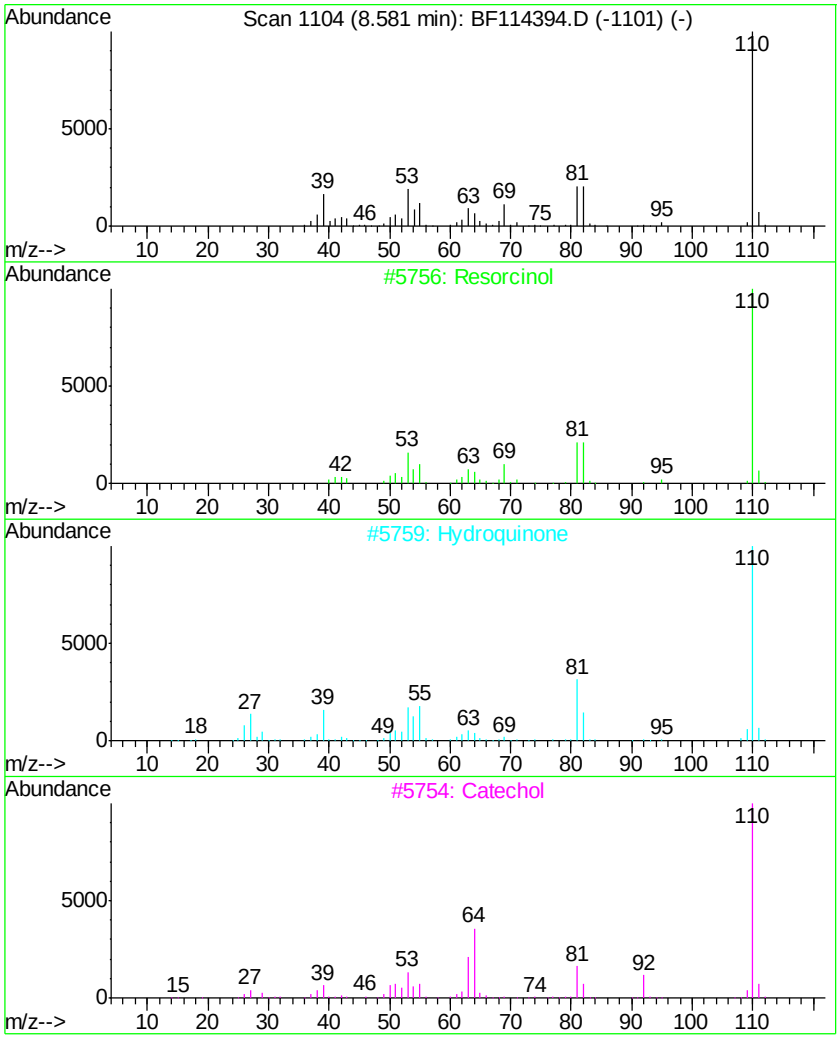
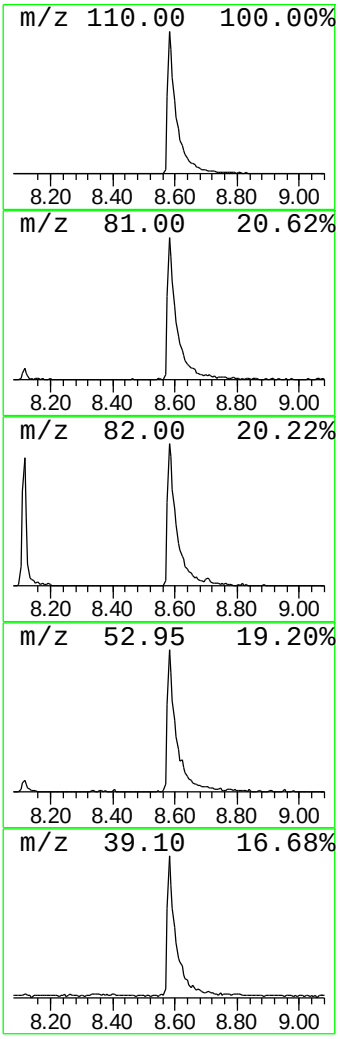
Peak Number 4 Resorcinol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.58	10.69 ng	946213	Naphthalene-d8	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Resorcinol	110	C6H6O2	000108-46-3	97
2	Hydroquinone	110	C6H6O2	000123-31-9	86
3	Catechol	110	C6H6O2	000120-80-9	58
4	3(2H)-Pyridazinone, 6-methyl-	110	C5H6N2O	013327-27-0	53
5	2(1H)-Pyridinone, 3-amino-	110	C5H6N2O	033630-99-8	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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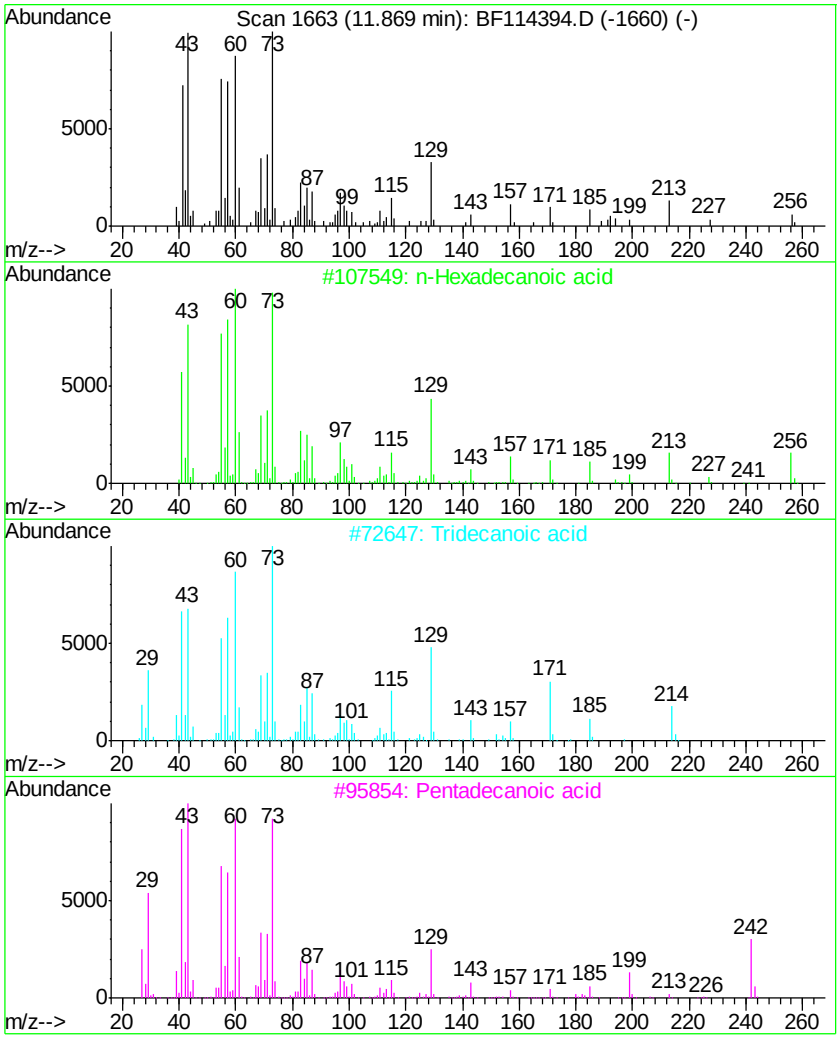
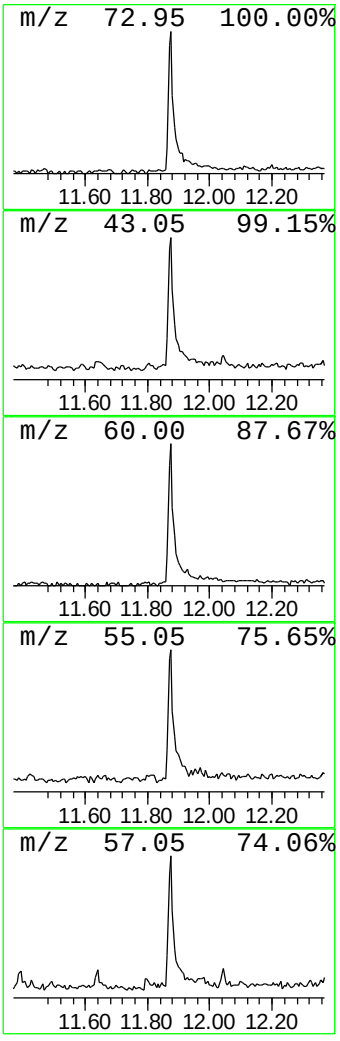
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.67 ng	285835	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	76





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Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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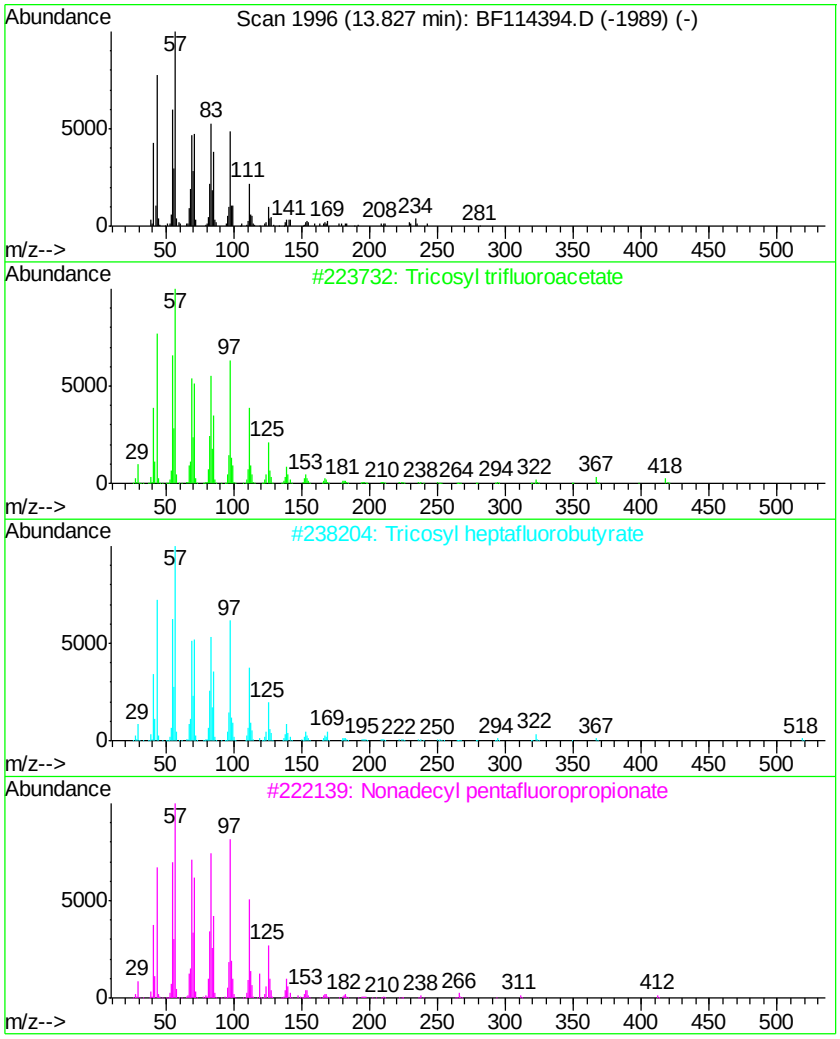
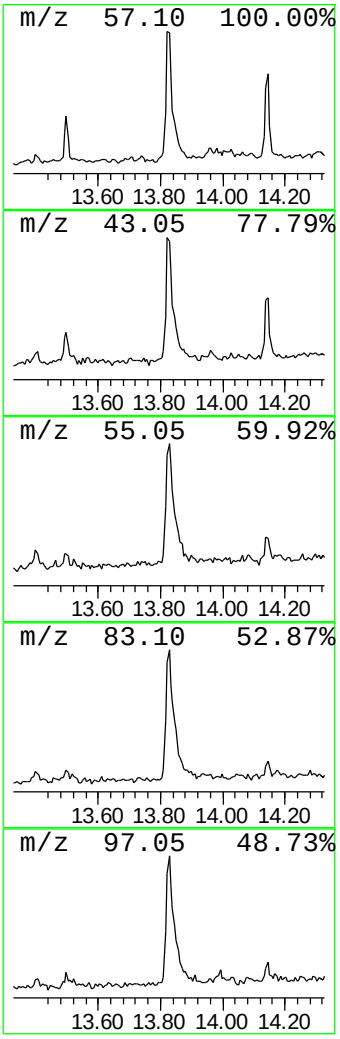
Peak Number 6 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.97 ng	453866	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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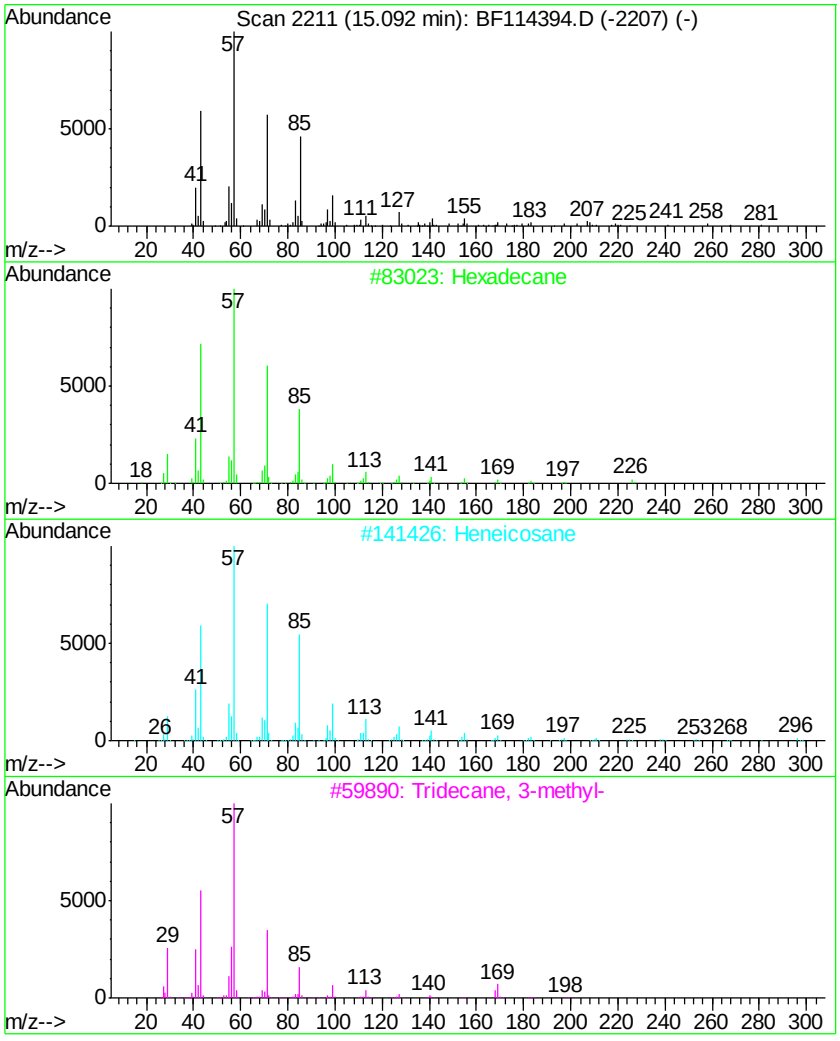
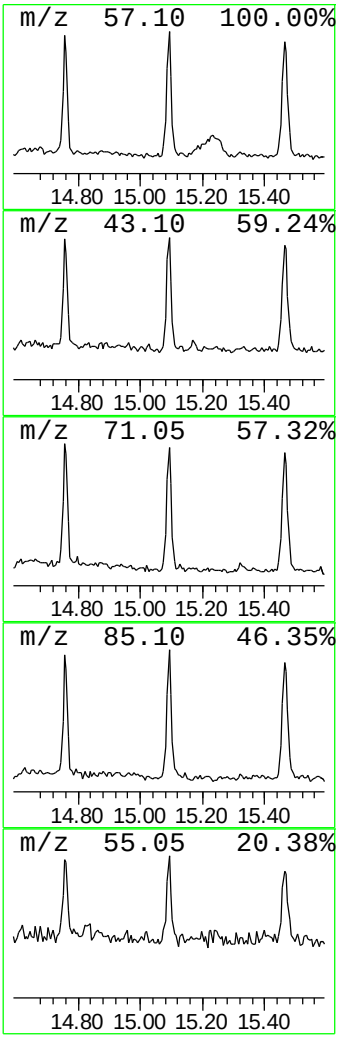
Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.35 ng	200130	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
4	Heptacosane	380	C27H56	000593-49-7	74
5	Decane, 3-methyl-	156	C11H24	013151-34-3	72





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Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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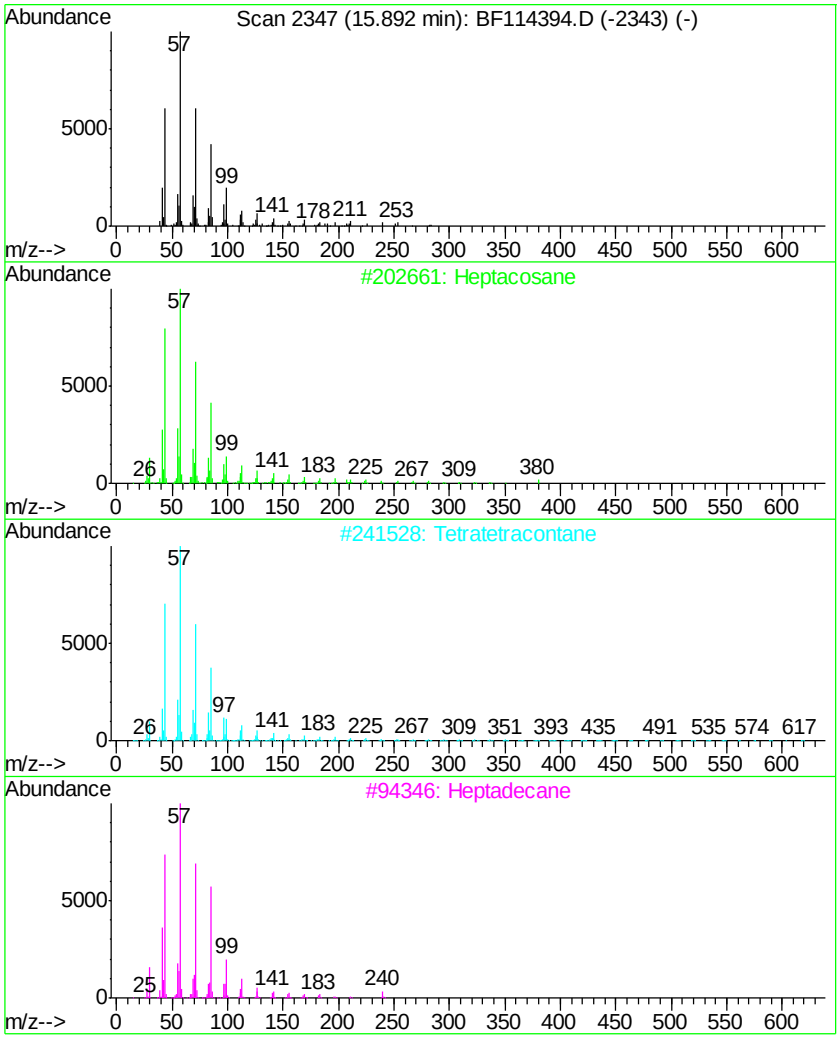
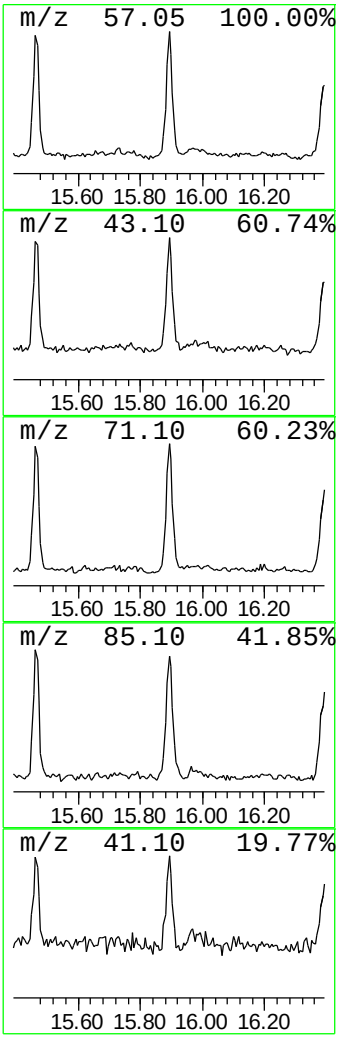
Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	2.52 ng	214498	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Heptadecane, 4-propyl-	282	C20H42	055044-10-5	86
5	Octacosane	394	C28H58	000630-02-4	81





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Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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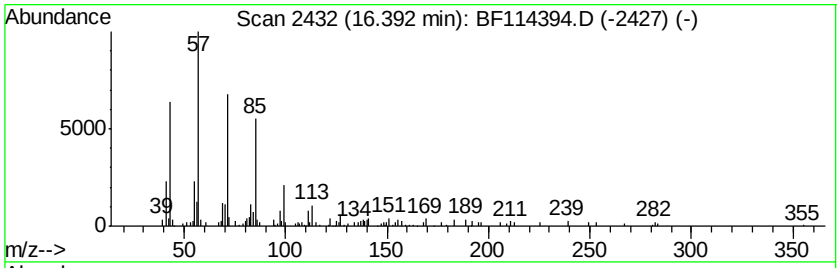
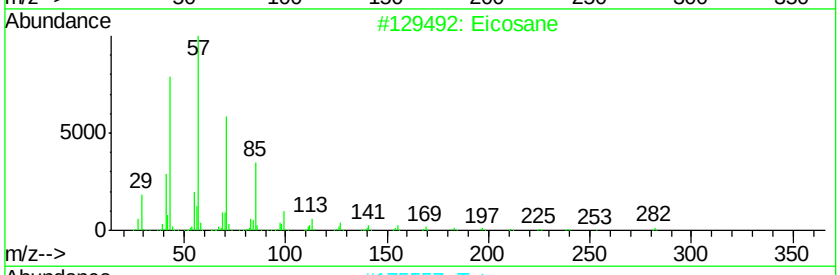
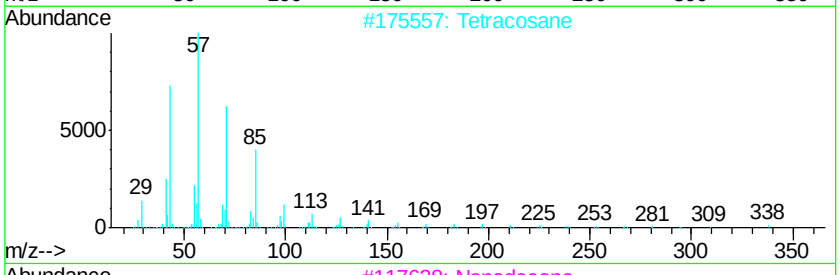
Peak Number 9 Eicosane Concentration Rank 9

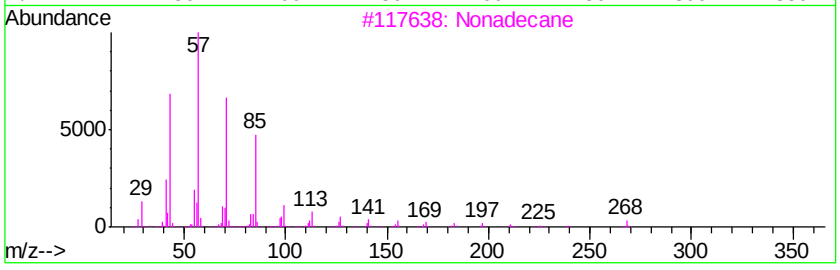
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.39	2.03 ng	172621	Perylene-d12	15.47

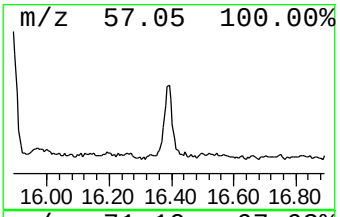
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Tetracosane	338	C24H50	000646-31-1	80
3	Nonadecane	268	C19H40	000629-92-5	80
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	58

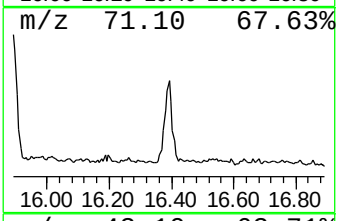


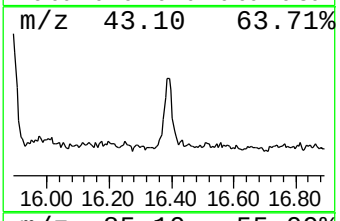


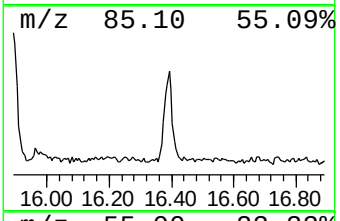


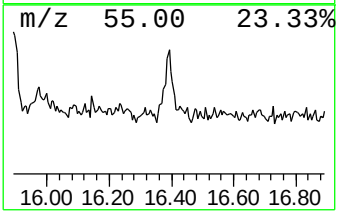












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114394.D
Acq On : 18 May 2019 16:37
Operator : JU/SJ
Sample : K2880-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 339-RBR-251608

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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...	2.13	28.1	ng	1950490	1	6.83	1390920	20.0
unknown6.62	6.62	87.9	ng	6114940	1	6.83	1390920	20.0
Resorcinol	8.58	10.7	ng	946213	2	8.12	1770970	20.0
n-Hexadecanoic acid	11.87	2.7	ng	285835	4	11.35	2138530	20.0
Tricosyl trifluor...	13.83	5.0	ng	453866	5	13.99	1826420	20.0
Hexadecane	15.09	2.4	ng	200130	6	15.47	1704520	20.0
Heptacosane	15.89	2.5	ng	214498	6	15.47	1704520	20.0
Eicosane	16.39	2.0	ng	172621	6	15.47	1704520	20.0