LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107588.D
Acq On : 23 Jul 2018 15:18
Operator : JU/SJ
Sample : J4062-25
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9

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-BF072018.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	5.207	484	488	505	rVB	786091	987397	17.50%	1.689%
2	5.601	551	555	590	rBV	4158889	5421010	96.08%	9.273%
3	6.607	721	726	745	rBV	4382357	5642404	100.00%	9.651%
4	6.748	745	750	769	rVB	5066025	5641808	99.99%	9.650%
5	6.972	785	788	811	rBV	1619018	1922420	34.07%	3.288%
6	7.131	811	815	844	rVB	4137869	4236911	75.09%	7.247%
7	7.537	880	884	905	rBV	3213484	3691425	65.42%	6.314%
8	8.254	1003	1006	1026	rBV	2173635	2496123	44.24%	4.270%
9	9.331	1185	1189	1198	rBV	5902038	5575476	98.81%	9.537%
10	9.725	1252	1256	1261	rBV	222999	214049	3.79%	0.366%
11	10.019	1302	1306	1317	rBV	2471689	2556300	45.31%	4.373%
12	10.425	1367	1375	1380	rBV2	56669	72484	1.28%	0.124%
13	10.807	1436	1440	1453	rBV	3341700	3778071	66.96%	6.462%
14	10.901	1454	1456	1466	rVB2	56024	97336	1.73%	0.166%
15	11.513	1556	1560	1562	rBV	2333167	2172541	38.50%	3.716%
16	11.536	1562	1564	1570	rVV	440458	471235	8.35%	0.806%
17	11.589	1570	1573	1577	rVB	61042	73892	1.31%	0.126%
18	12.019	1642	1646	1649	rBV2	445461	448528	7.95%	0.767%
19	12.042	1649	1650	1656	rVB2	110243	162816	2.89%	0.279%
20	12.124	1661	1664	1667	rBV2	74469	94233	1.67%	0.161%
21	12.730	1763	1767	1773	rBV	509957	538679	9.55%	0.921%
22	12.960	1800	1806	1812	rBV	520737	647128	11.47%	1.107%
23	13.095	1825	1829	1839	rBV	4740897	4277890	75.82%	7.317%
24	13.283	1855	1861	1863	rBV4	77009	113703	2.02%	0.194%
25	13.395	1876	1880	1882	rBV2	44503	59102	1.05%	0.101%
26	13.648	1920	1923	1926	rBV	84252	80534	1.43%	0.138%
27	13.977	1975	1979	1982	rBV2	645135	675163	11.97%	1.155%
28	14.160	2005	2010	2013	rBV	2016603	2236214	39.63%	3.825%
29	14.295	2030	2033	2039	rBV	131132	155395	2.75%	0.266%
30	14.607	2083	2086	2091	rVB3	221195	253655	4.50%	0.434%
31	14.924	2137	2140	2143	rBV	155890	143711	2.55%	0.246%
32	15.083	2164	2167	2173	rVB4	115346	144886	2.57%	0.248%
33	15.236	2190	2193	2197	rBV2	168573	294047	5.21%	0.503%
34	15.283	2198	2201	2204	rVB	189839	231304	4.10%	0.396%

LSC Area Percent Report

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Instrument : BNA_F
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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-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.560	2246	2248	2254	rVB	119032	167710	2.97%	0.287%
36	15.630	2257	2260	2266	rVV	140921	201247	3.57%	0.344%
37	15.701	2266	2272	2286	rVV	1394072	2256481	39.99%	3.860%
38	16.154	2346	2349	2353	rVB	169083	228444	4.05%	0.391%

Sum of corrected areas: 58461752

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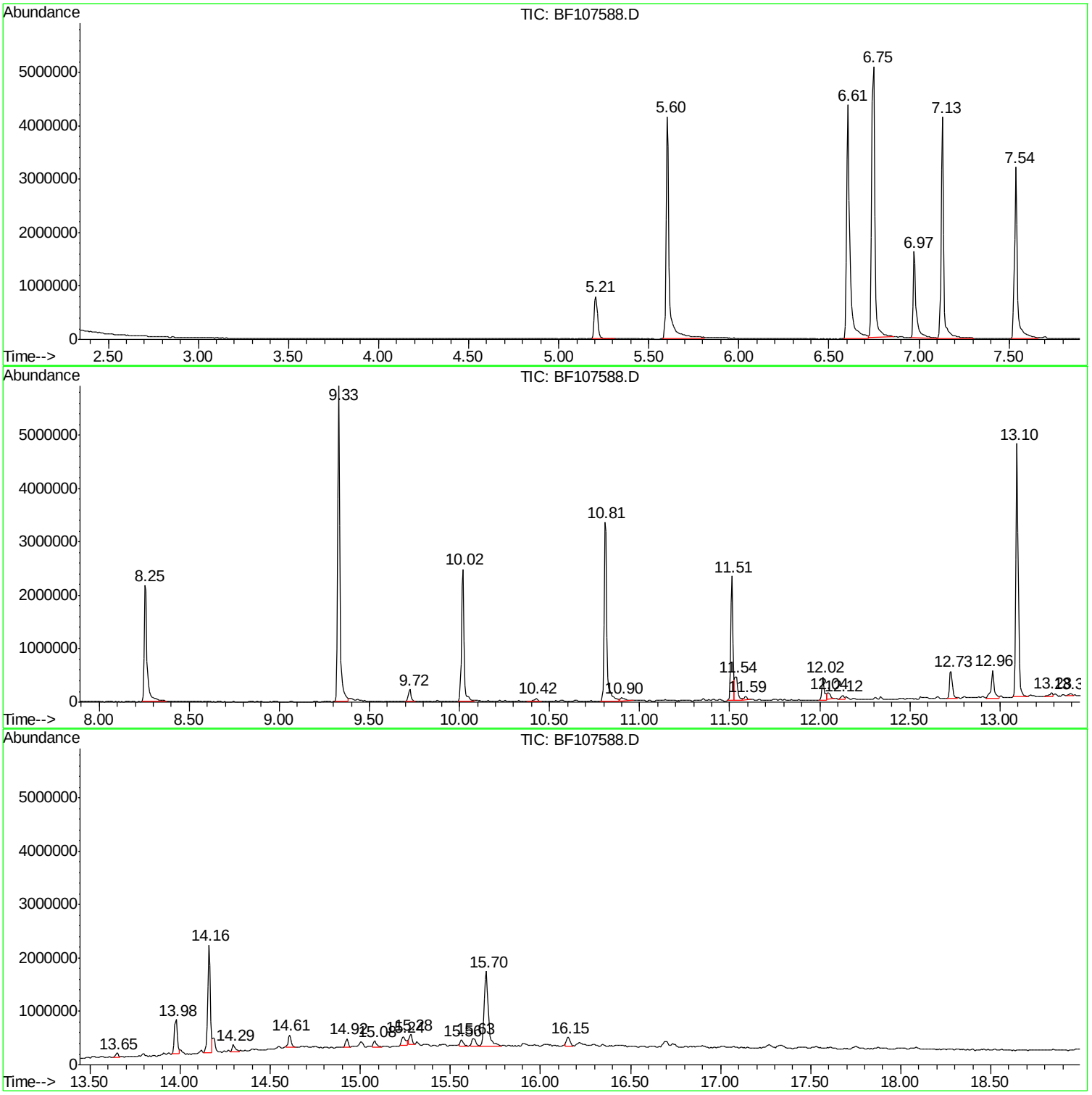
Instrument :
BNA_F
ClientSampleId :
TP-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

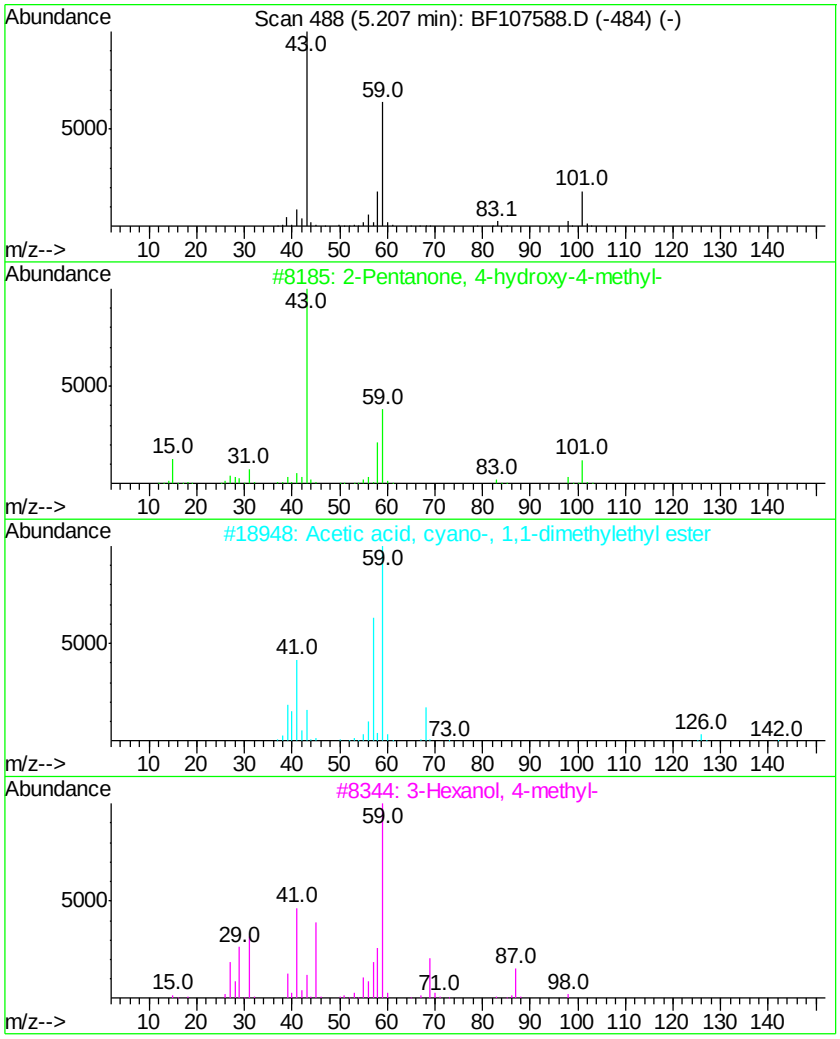
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

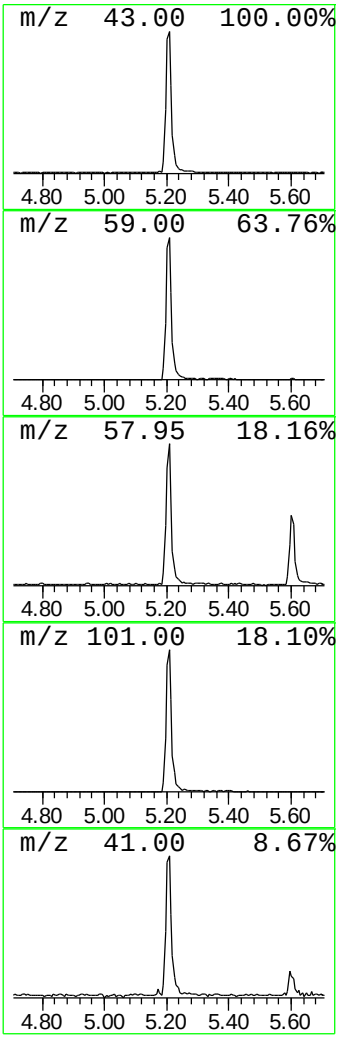
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	10.27 ng	987397	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J4062-25
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
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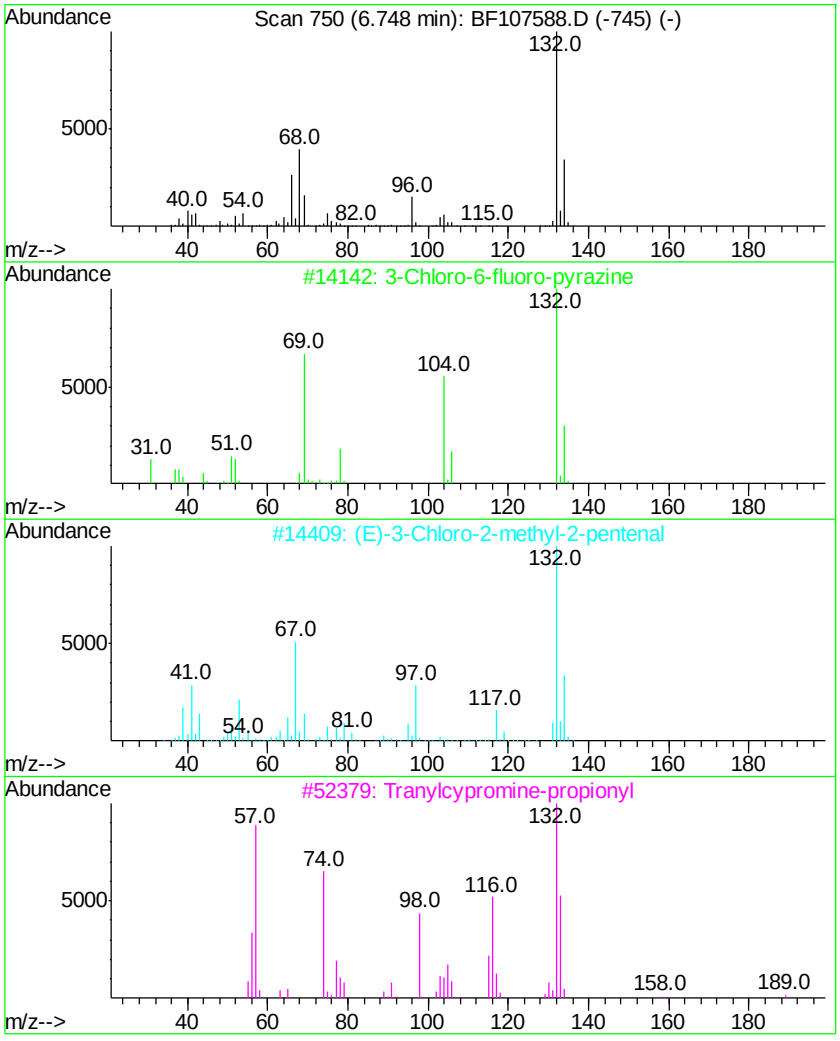
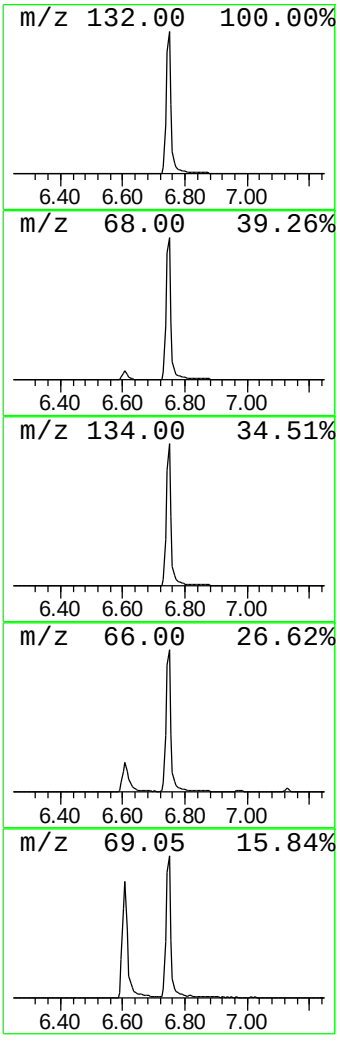
****

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	58.69 ng	5641810	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
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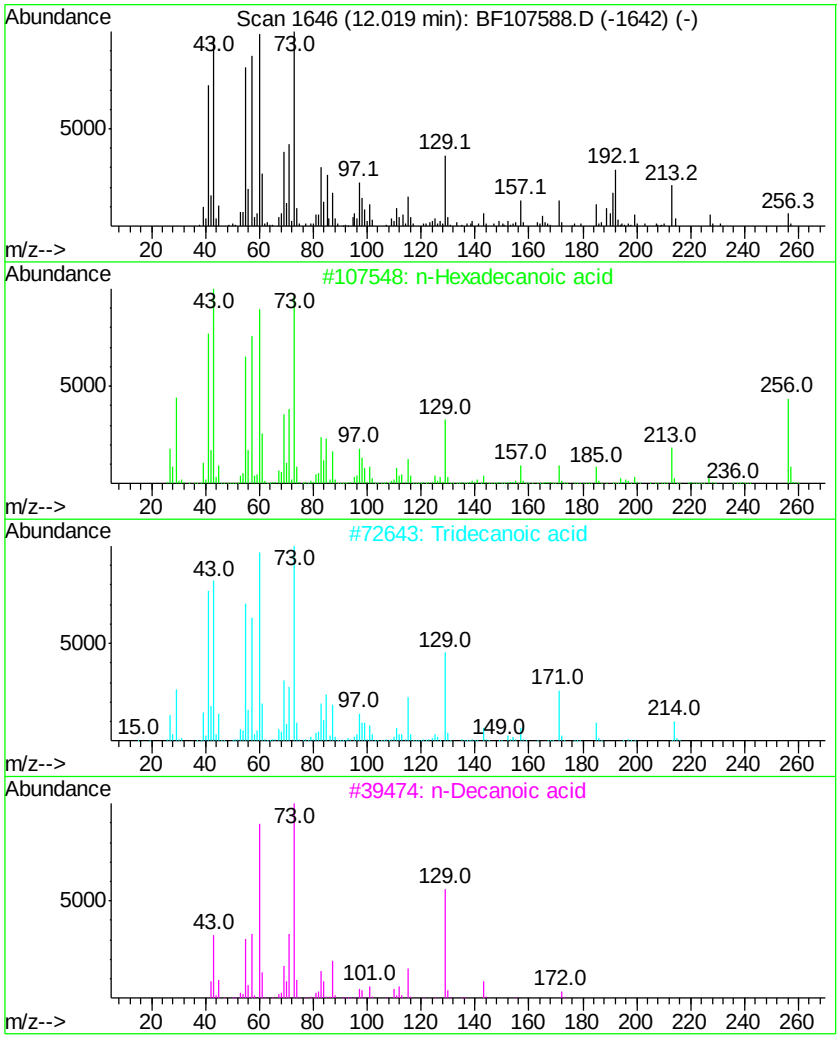
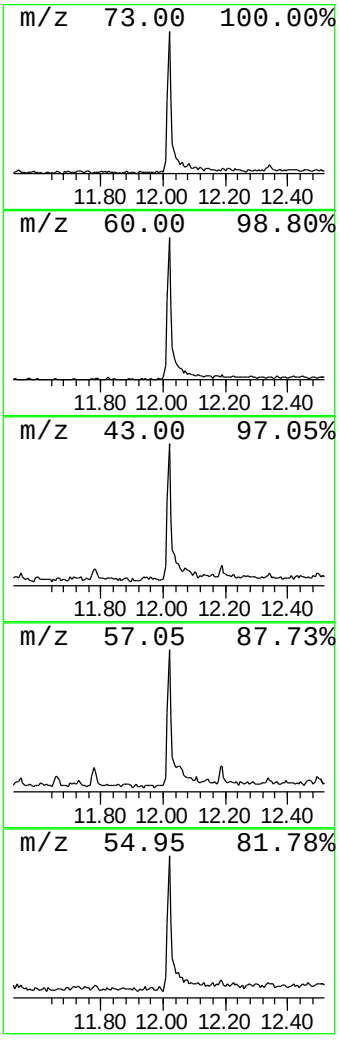
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	4.13 ng	448528	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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TIC Library : C:\DATABASE\NIST11.L
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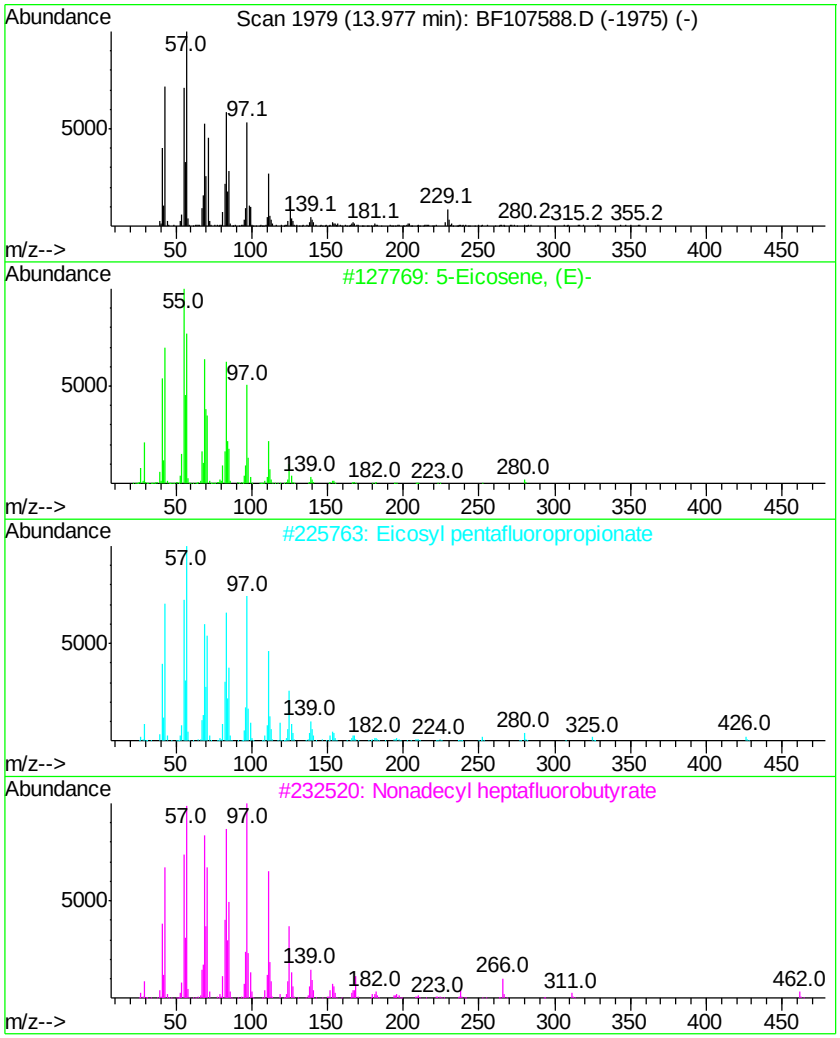
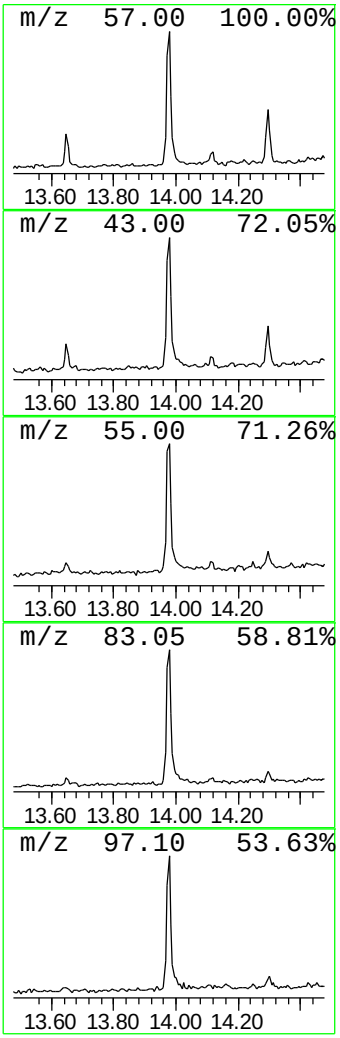
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	6.04 ng	675163	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
3	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : TP-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

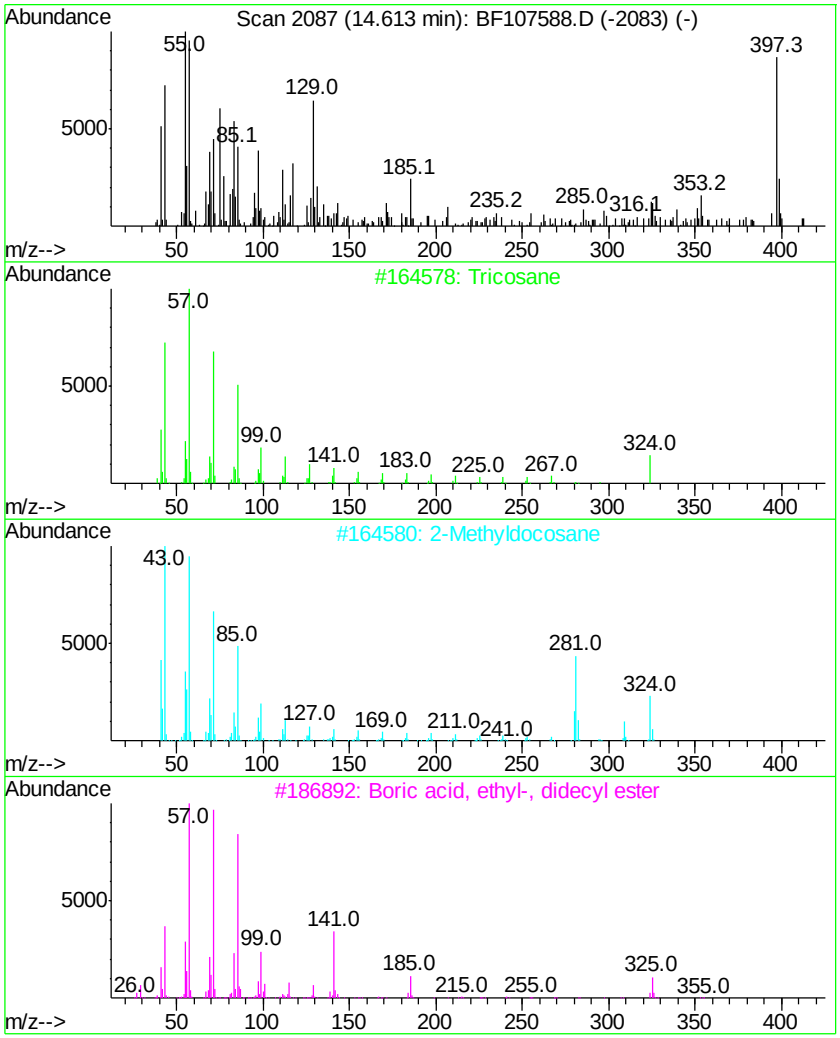
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

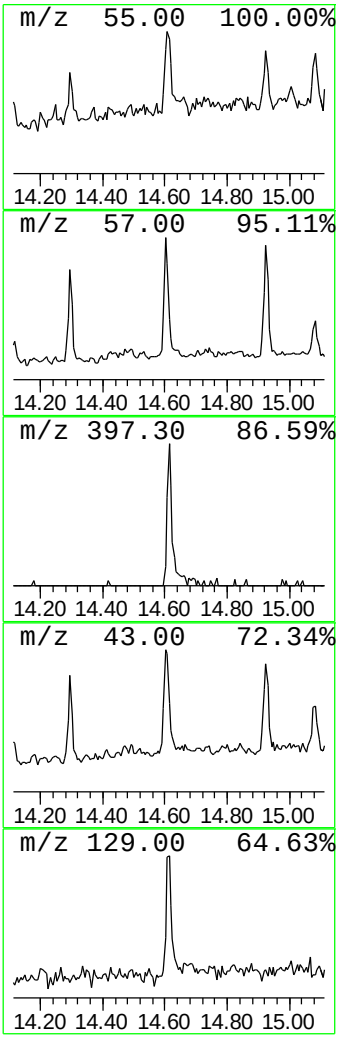
****

Peak Number 6 Tricosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	2.27 ng	253655	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	55
2	2-Methyldocosane	324	C23H48	001560-81-2	37
3	Boric acid, ethyl-, didecyl ester	354	C22H47BO2	1000152-34-4	25
4	2H-Isoindole-5-carboxamide, 2-(2...	394	C21H18N2O6	294892-21-0	9
5	Pseudokryptogenin	412	C27H40O3	065682-56-6	9





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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

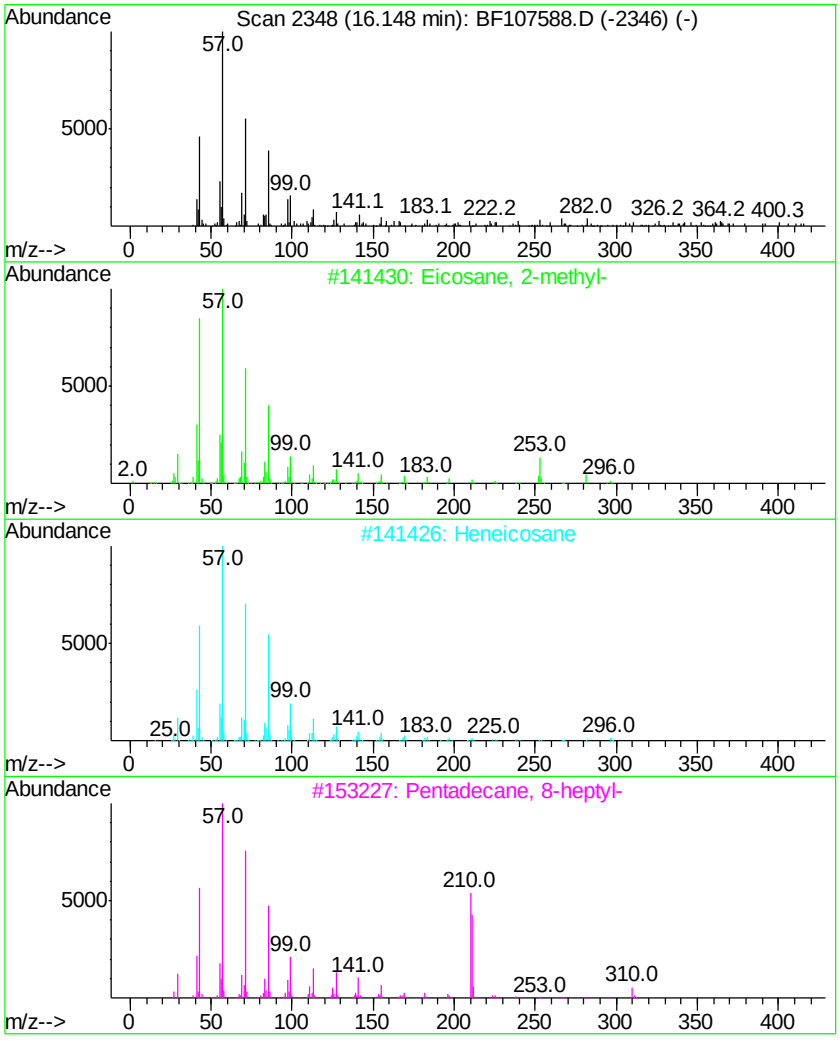
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

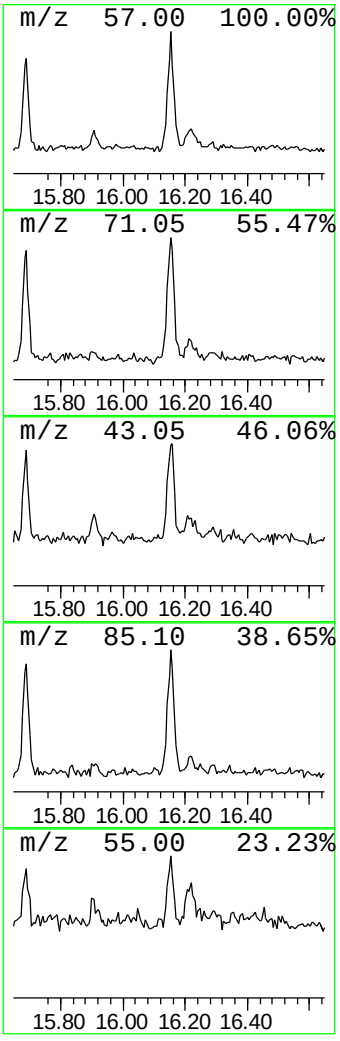
****

Peak Number 7 Eicosane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	2.02 ng	228444	Perylene-d12	15.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 2-methyl-	296	C21H44	001560-84-5	89
2	Heneicosane	296	C21H44	000629-94-7	89
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	83
4	Hexacosane	366	C26H54	000630-01-3	83
5	Dodecane, 4,9-dipropyl-	254	C18H38	003054-63-5	80





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.21	10.3	ng	987397	1	6.97	1922420	20.0
unknown6.75	6.75	58.7	ng	5641810	1	6.97	1922420	20.0
n-Hexadecanoic acid	12.02	4.1	ng	448528	4	11.51	2172540	20.0
5-Eicosene, (E)-	13.98	6.0	ng	675163	5	14.16	2236210	20.0
Tricosane	14.61	2.3	ng	253655	5	14.16	2236210	20.0
Eicosane, 2-methyl-	16.15	2.0	ng	228444	6	15.70	2256480	20.0