

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120319\
 Data File : BF118073.D
 Acq On : 3 Dec 2019 20:20
 Operator : JU
 Sample : K6069-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF111319.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	2.140	3	9	15	rBV	628790	825482	21.97%	2.622%
2	2.510	62	72	79	rVB	78759	119223	3.17%	0.379%
3	4.604	424	428	432	rBV	51930	56132	1.49%	0.178%
4	5.081	502	509	524	rBV	388830	488536	13.00%	1.552%
5	5.493	574	579	582	rBV	2456324	2316602	61.66%	7.358%
6	6.504	746	751	767	rVB	2413820	2568176	68.36%	8.157%
7	6.645	770	775	778	rBV	3063113	2655262	70.68%	8.433%
8	6.875	810	814	818	rBV	1066275	794937	21.16%	2.525%
9	7.034	837	841	844	rBV	2578291	2145681	57.11%	6.815%
10	7.439	905	910	913	rBV	1719817	1612518	42.92%	5.121%
11	8.163	1029	1033	1036	rBV	1233589	1032545	27.48%	3.279%
12	9.239	1212	1216	1220	rBV	3701418	3233271	86.06%	10.269%
13	9.633	1279	1283	1288	rBV	449361	364360	9.70%	1.157%
14	9.928	1328	1333	1336	rBV	1362338	1257633	33.48%	3.994%
15	10.716	1463	1467	1478	rBV	2424868	2197752	58.50%	6.980%
16	11.416	1582	1586	1590	rBV	1531637	1368515	36.43%	4.346%
17	11.480	1594	1597	1603	rVB4	40230	45738	1.22%	0.145%
18	11.939	1670	1675	1678	rBV	212047	195800	5.21%	0.622%
19	11.975	1678	1681	1685	rVB	309805	265419	7.07%	0.843%
20	12.633	1791	1793	1799	rBV	62459	57174	1.52%	0.182%
21	12.727	1805	1809	1814	rBV	66278	78609	2.09%	0.250%
22	12.863	1828	1832	1837	rBV2	53568	95244	2.54%	0.302%
23	13.010	1852	1857	1860	rBV	4327300	3756812	100.00%	11.932%
24	13.439	1927	1930	1933	rBV3	37648	42670	1.14%	0.136%
25	13.469	1933	1935	1942	rVB4	70354	90781	2.42%	0.288%
26	13.898	2001	2008	2021	rBV2	379765	522848	13.92%	1.661%
27	14.068	2033	2037	2040	rBV	1263153	1133246	30.17%	3.599%
28	14.221	2060	2063	2067	rBV	84384	93673	2.49%	0.298%
29	14.533	2113	2116	2122	rBV2	132261	159710	4.25%	0.507%
30	14.845	2166	2169	2172	rVB	95597	90809	2.42%	0.288%
31	14.921	2179	2182	2186	rVB	95343	94749	2.52%	0.301%
32	15.192	2224	2228	2231	rBV	135439	169674	4.52%	0.539%
33	15.563	2285	2291	2307	rVB	796905	1190918	31.70%	3.782%
34	16.033	2367	2371	2376	rVB2	102408	152330	4.05%	0.484%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.092	2377	2381	2392	rVB2	39568	76606	2.04%	0.243%
36	16.286	2411	2414	2423	rVB10	27330	48184	1.28%	0.153%
37	16.557	2455	2460	2467	rVB2	50955	88333	2.35%	0.281%

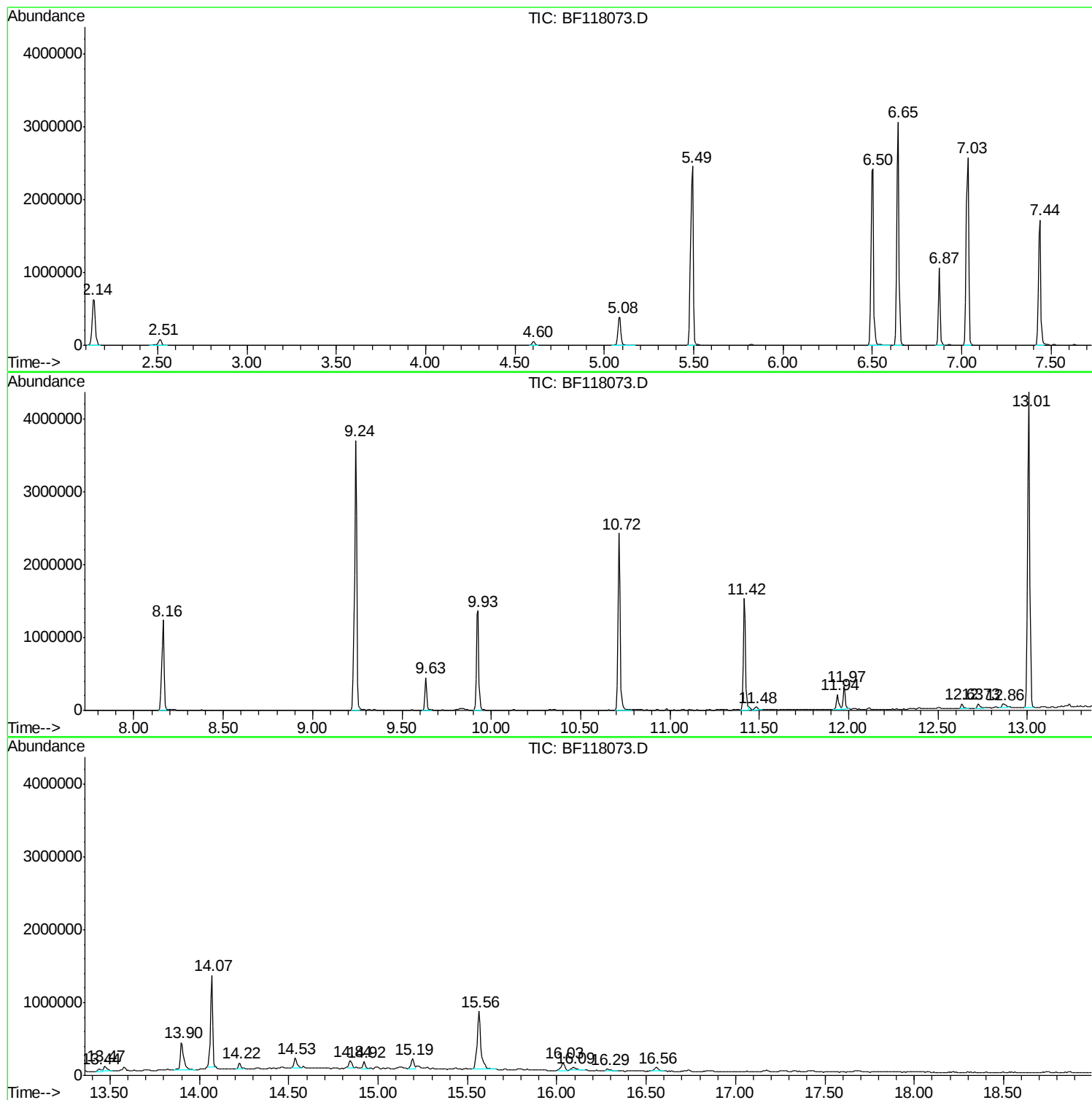
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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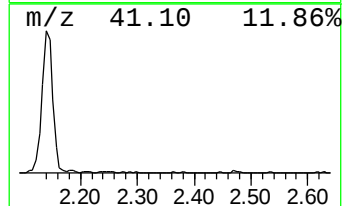
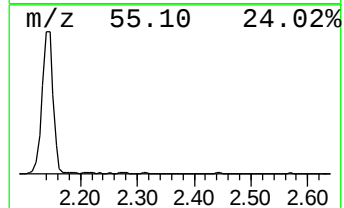
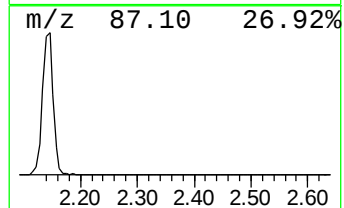
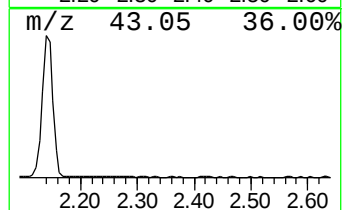
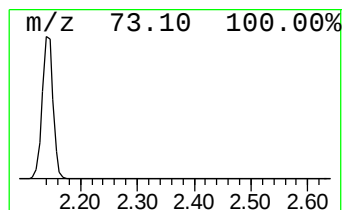
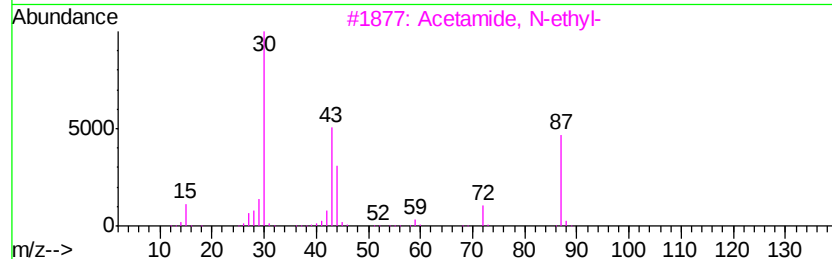
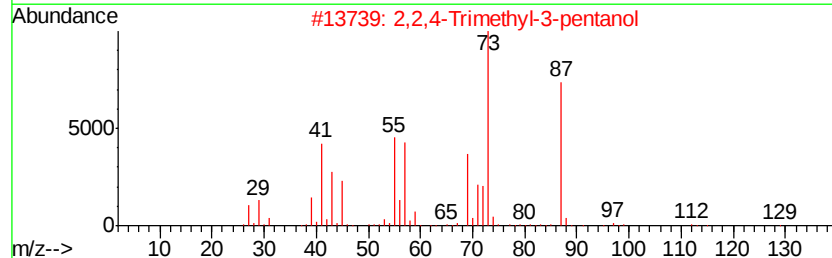
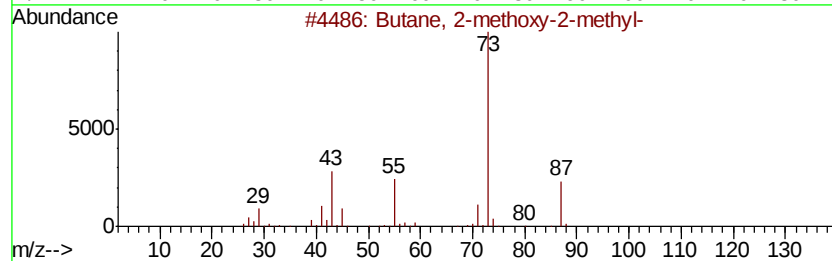
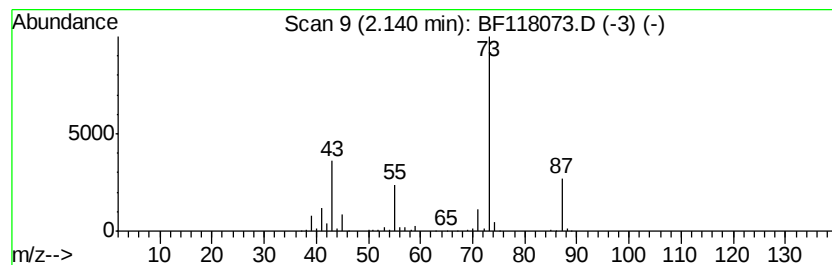
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	20.77 ng	825482	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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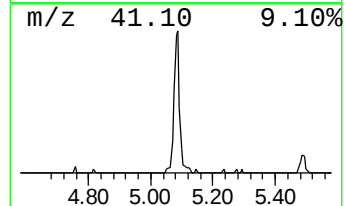
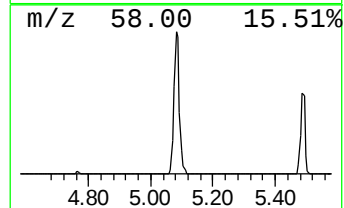
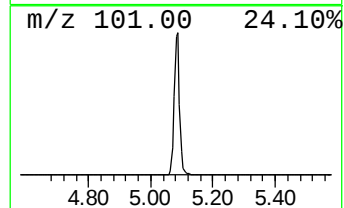
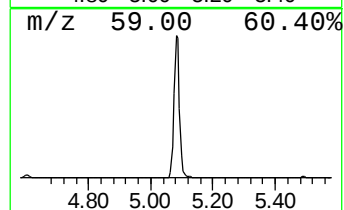
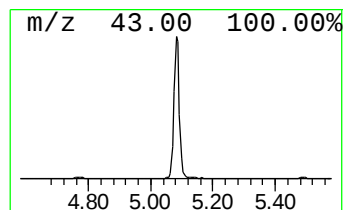
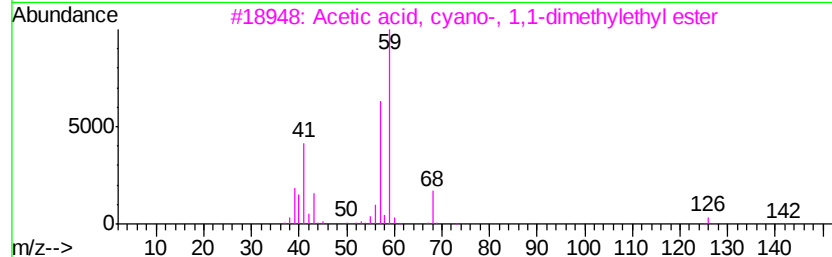
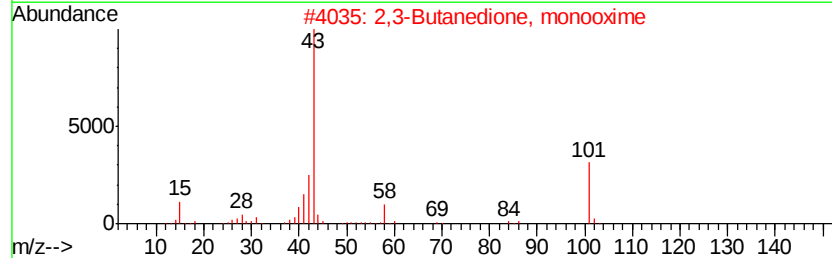
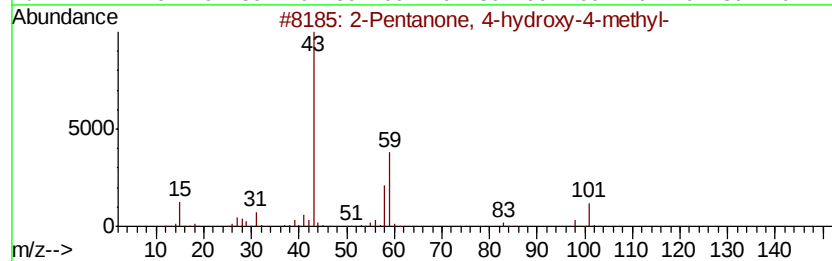
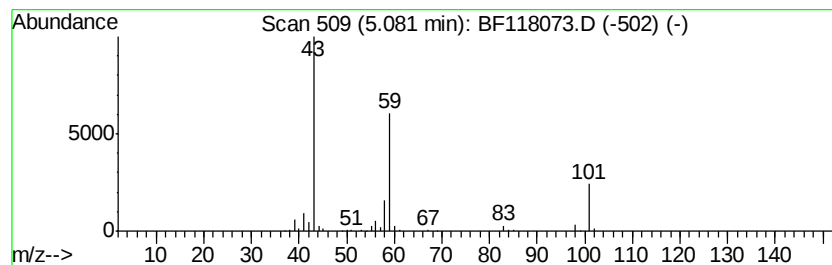
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	12.29 ng	488536	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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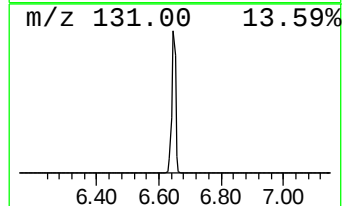
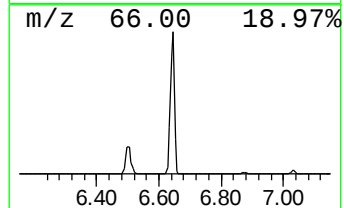
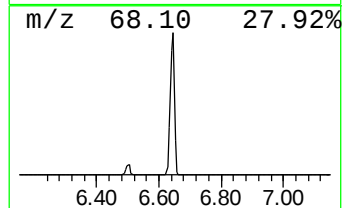
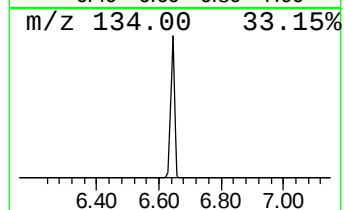
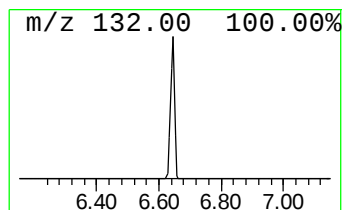
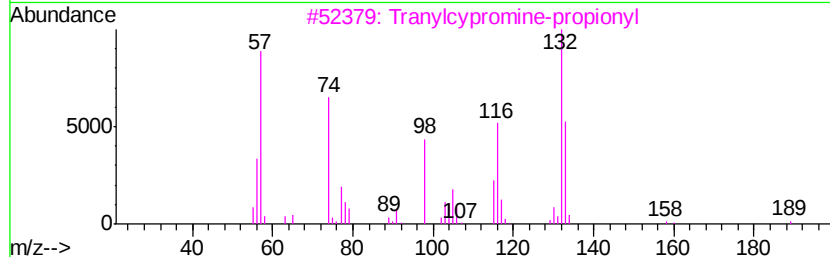
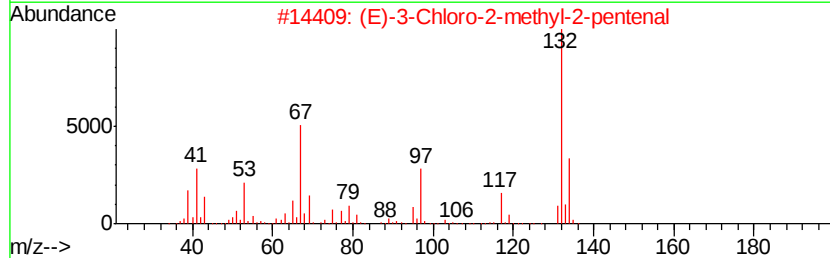
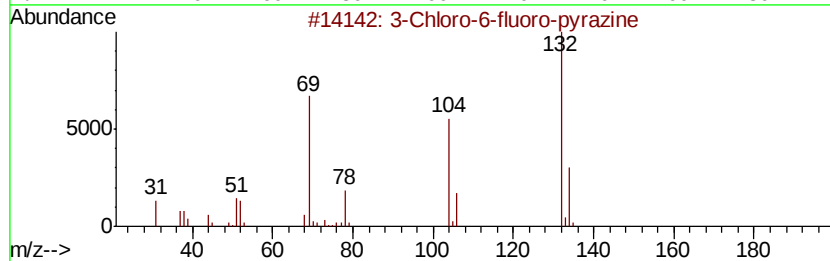
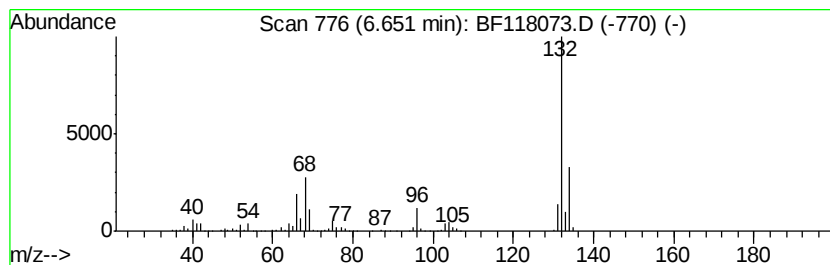
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	66.80 ng	2655260	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
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



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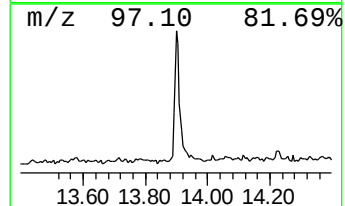
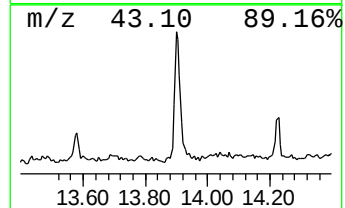
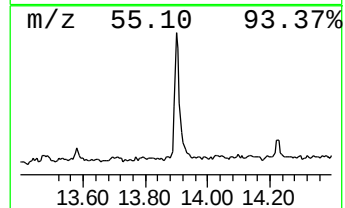
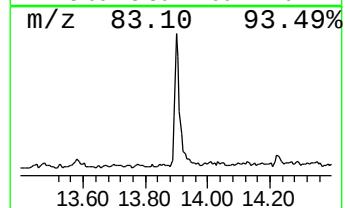
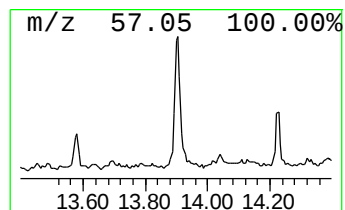
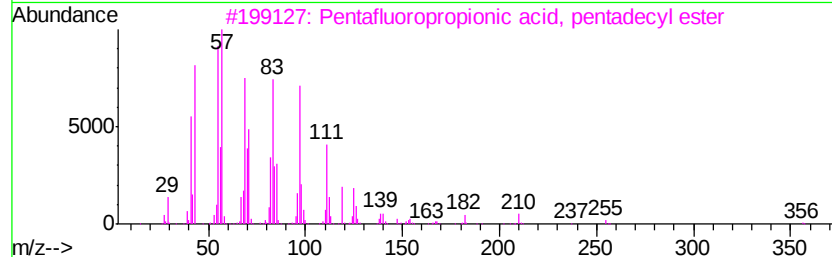
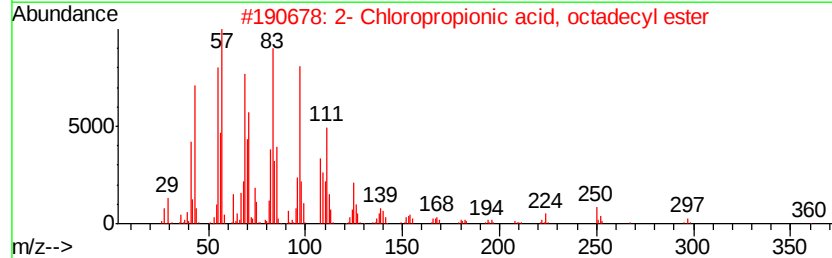
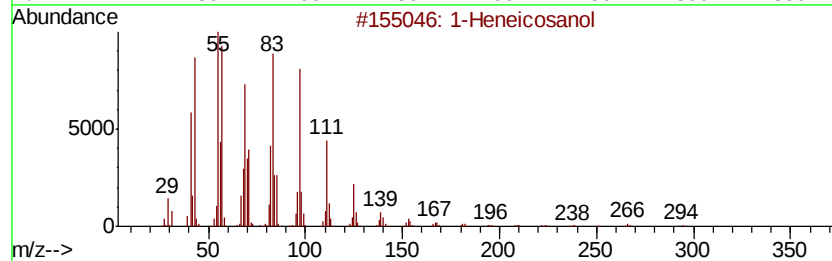
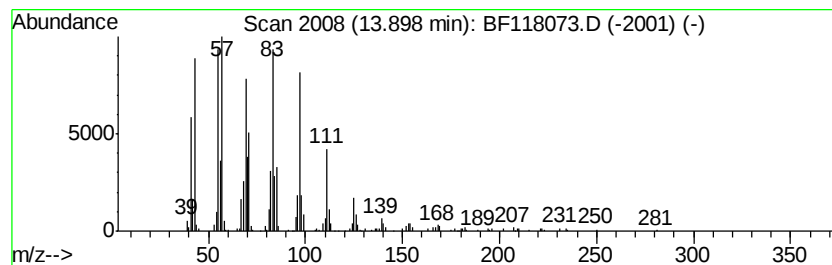
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.90	9.23 ng	522848	Chrysene-d12	14.07		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



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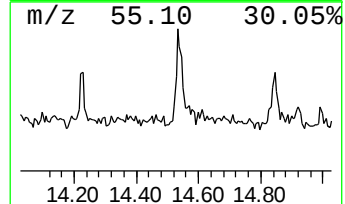
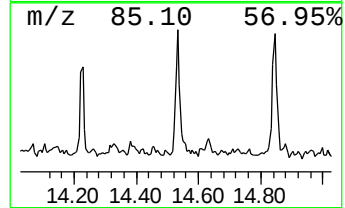
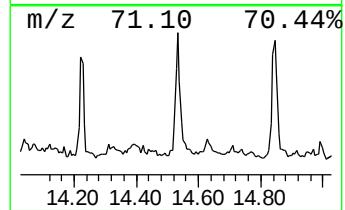
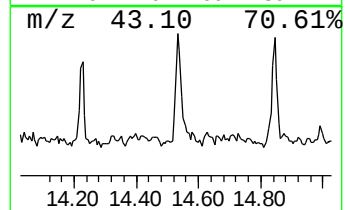
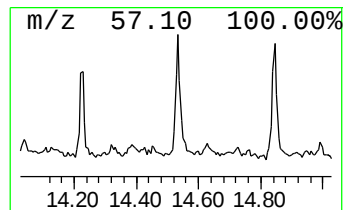
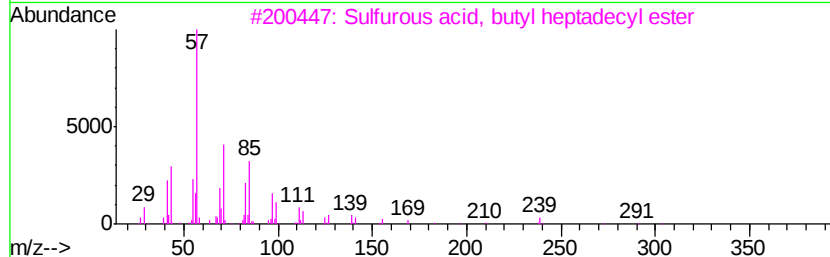
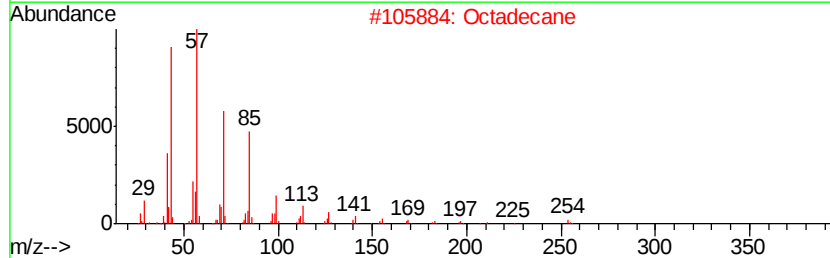
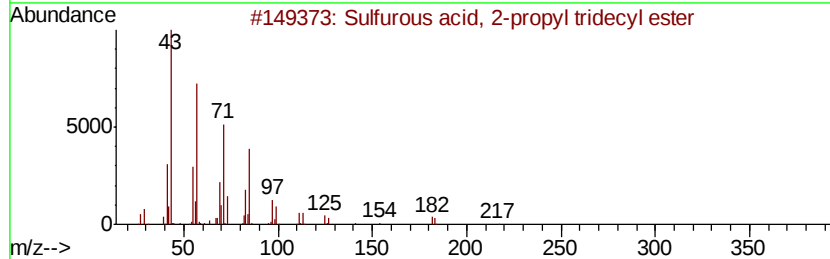
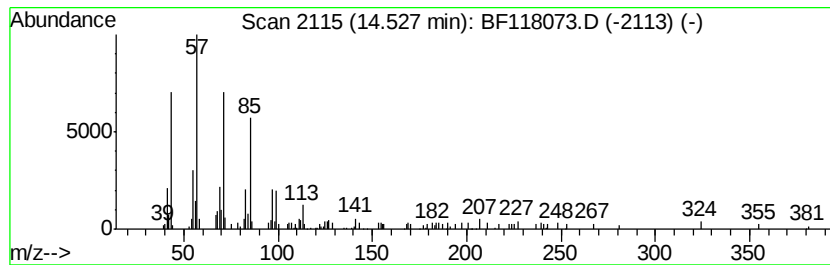
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.82 ng	159710	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-propyl tridecyl...	306	C16H34O3S	1000309-12-4	90
2		Octadecane	254	C18H38	000593-45-3	87
3		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	74
4		Hexacosane	366	C26H54	000630-01-3	72
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120319\
Data File : BF118073.D
Acq On : 3 Dec 2019 20:20
Operator : JU
Sample : K6069-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4

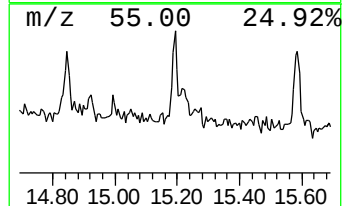
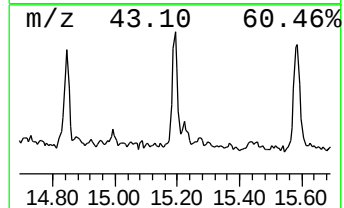
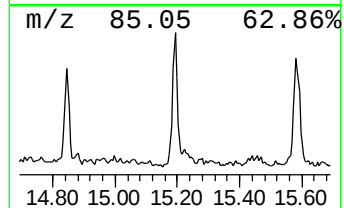
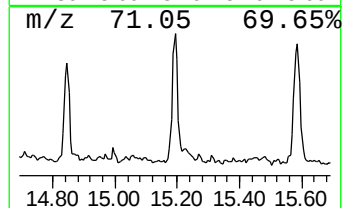
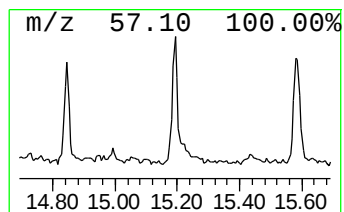
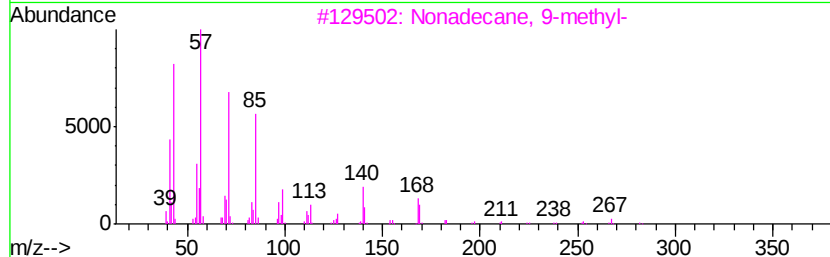
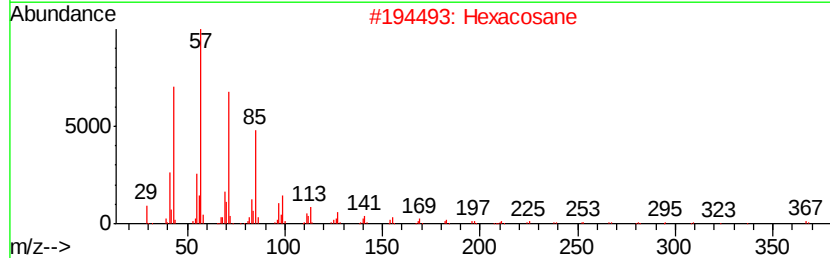
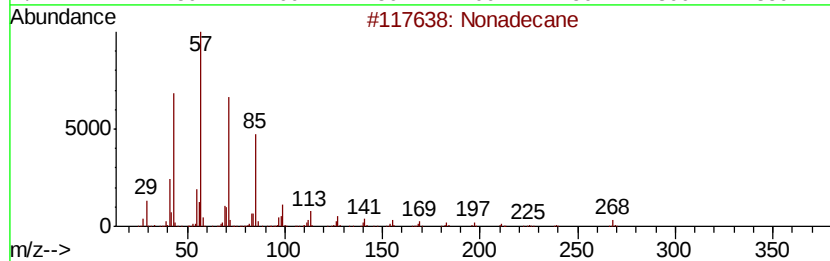
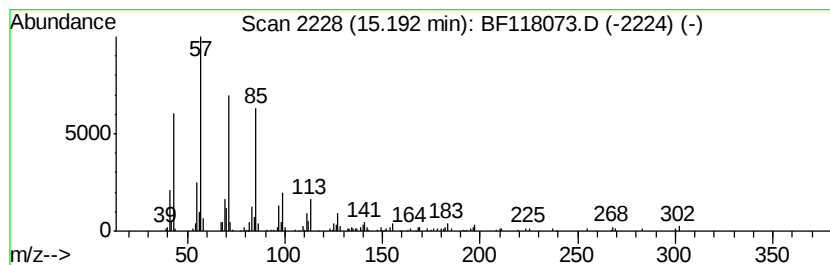
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	2.85 ng	169674	Perylene-d12	15.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	94
2	Hexacosane		366	C26H54	000630-01-3	91
3	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	91
4	Pentacosane		352	C25H52	000629-99-2	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120319\
Data File : BF118073.D
Acq On : 3 Dec 2019 20:20
Operator : JU
Sample : K6069-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4

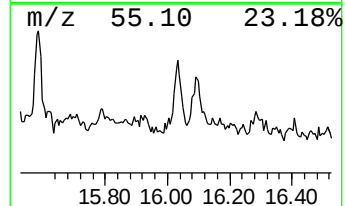
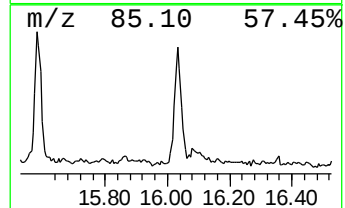
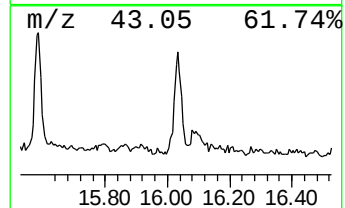
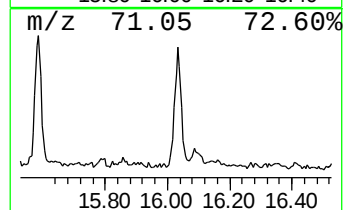
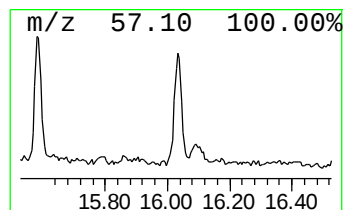
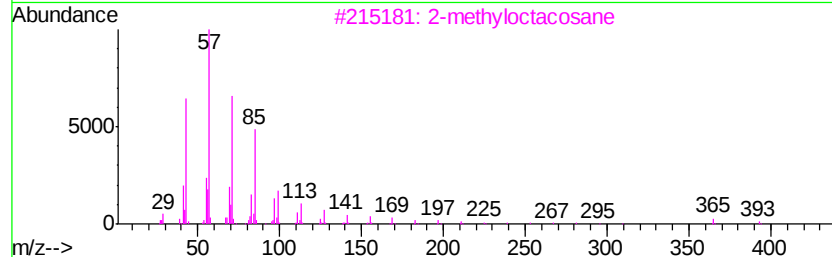
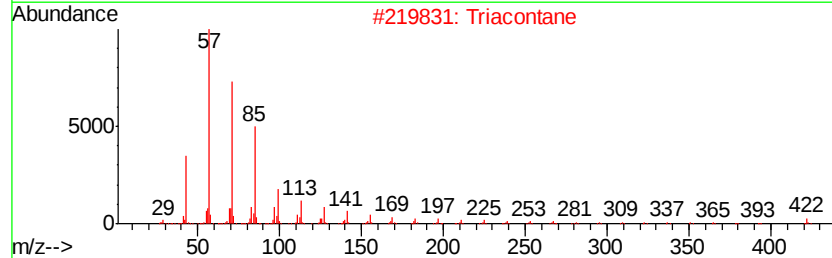
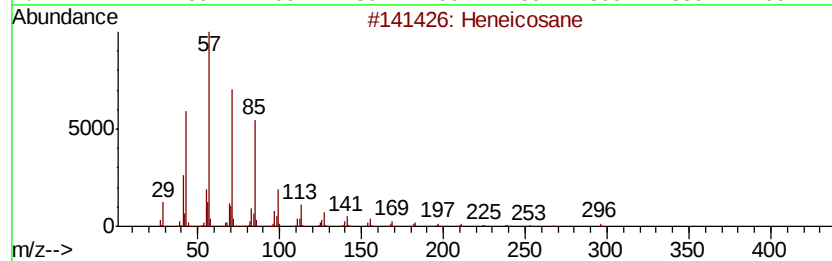
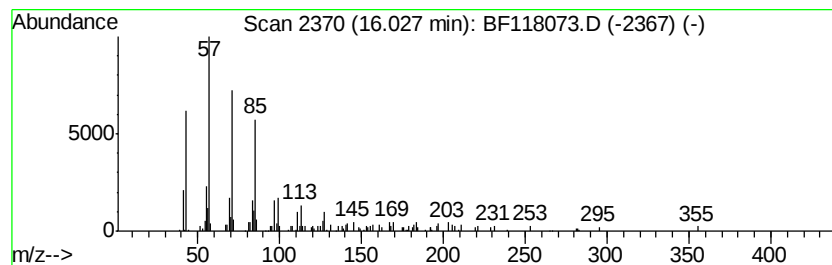
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.56 ng	152330	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Triacontane	422	C30H62	000638-68-6	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptacosane	380	C27H56	000593-49-7	90
5		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF120319\
Data File : BF118073.D
Acq On : 3 Dec 2019 20:20
Operator : JU
Sample : K6069-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.14	20.8	ng	825482	1	6.87	794937	20.0
2-Pentanone, 4-hy...	5.08	12.3	ng	488536	1	6.87	794937	20.0
unknown6.65	6.65	66.8	ng	2655260	1	6.87	794937	20.0
1-Heneicosanol	13.90	9.2	ng	522848	5	14.07	1133250	20.0
Sulfurous acid, 2...	14.53	2.8	ng	159710	5	14.07	1133250	20.0
Nonadecane	15.19	2.9	ng	169674	6	15.56	1190920	20.0
Heneicosane	16.03	2.6	ng	152330	6	15.56	1190920	20.0