

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
 Data File : BF118412.D
 Acq On : 31 Dec 2019 18:27
 Operator : JU
 Sample : K6465-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GP-9-(1-3)

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-BF122419.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	5.063	502	506	521	rVB	209120	265779	13.67%	1.424%
2	5.475	572	576	600	rBV	1572243	1539572	79.20%	8.250%
3	6.492	745	749	768	rBV	1647826	1650040	84.89%	8.842%
4	6.628	768	772	775	rBV	2026798	1795537	92.37%	9.621%
5	6.851	807	810	816	rBV	591197	473734	24.37%	2.539%
6	7.010	833	837	840	rBV	1643115	1350008	69.45%	7.234%
7	7.416	902	906	919	rBV	940695	1010187	51.97%	5.413%
8	8.139	1025	1029	1047	rBV	636407	620704	31.93%	3.326%
9	9.216	1208	1212	1228	rBV	2083836	1943813	100.00%	10.416%
10	9.616	1276	1280	1290	rBV	146523	151440	7.79%	0.811%
11	9.898	1325	1328	1343	rBV	669397	719304	37.00%	3.854%
12	10.698	1460	1464	1479	rBV	1296284	1297316	66.74%	6.952%
13	11.398	1579	1583	1585	rBV	637712	616960	31.74%	3.306%
14	11.422	1585	1587	1592	rVV	147104	136374	7.02%	0.731%
15	11.474	1592	1596	1602	rVB	28577	34718	1.79%	0.186%
16	11.621	1617	1621	1623	rBV3	15040	22227	1.14%	0.119%
17	11.916	1667	1671	1680	rBV3	165677	189343	9.74%	1.015%
18	12.016	1685	1688	1690	rBV	23533	22790	1.17%	0.122%
19	12.616	1787	1790	1800	rBV	243296	240038	12.35%	1.286%
20	12.704	1802	1805	1812	rVB4	34501	46804	2.41%	0.251%
21	12.845	1823	1829	1835	rVB	207377	209045	10.75%	1.120%
22	12.921	1839	1842	1845	rVB	47092	45393	2.34%	0.243%
23	12.986	1848	1853	1856	rBV	1749969	1554080	79.95%	8.328%
24	13.204	1888	1890	1895	rVB	49526	44305	2.28%	0.237%
25	13.286	1901	1904	1908	rVB3	21437	25732	1.32%	0.138%
26	13.551	1945	1949	1953	rBV2	46265	53728	2.76%	0.288%
27	13.880	1998	2005	2009	rBV3	215778	301806	15.53%	1.617%
28	14.015	2025	2028	2030	rBV	44839	42700	2.20%	0.229%
29	14.051	2030	2034	2037	rVV2	632289	678355	34.90%	3.635%
30	14.080	2037	2039	2048	rVB	97819	113627	5.85%	0.609%
31	14.198	2056	2059	2063	rBV3	29742	42002	2.16%	0.225%
32	14.504	2108	2111	2117	rBV3	56269	95301	4.90%	0.511%
33	14.810	2161	2163	2173	rVB	71141	89676	4.61%	0.481%
34	14.957	2185	2188	2194	rVB6	26843	41821	2.15%	0.224%

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GP-9-(1-3)

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35	15.110	2210	2214	2217	rBV	88244	135009	6.95%	0.723%
36	15.157	2219	2222	2225	rVB	71816	89039	4.58%	0.477%
37	15.486	2275	2278	2282	rVB	88337	102317	5.26%	0.548%
38	15.551	2283	2289	2302	rBV	421371	652534	33.57%	3.497%
39	15.986	2359	2363	2367	rVB	58515	93275	4.80%	0.500%
40	16.051	2372	2374	2382	rVB8	41741	70193	3.61%	0.376%
41	16.498	2447	2450	2453	rVB2	24338	25303	1.30%	0.136%
42	18.415	2770	2776	2777	rBV6	17262	29849	1.54%	0.160%

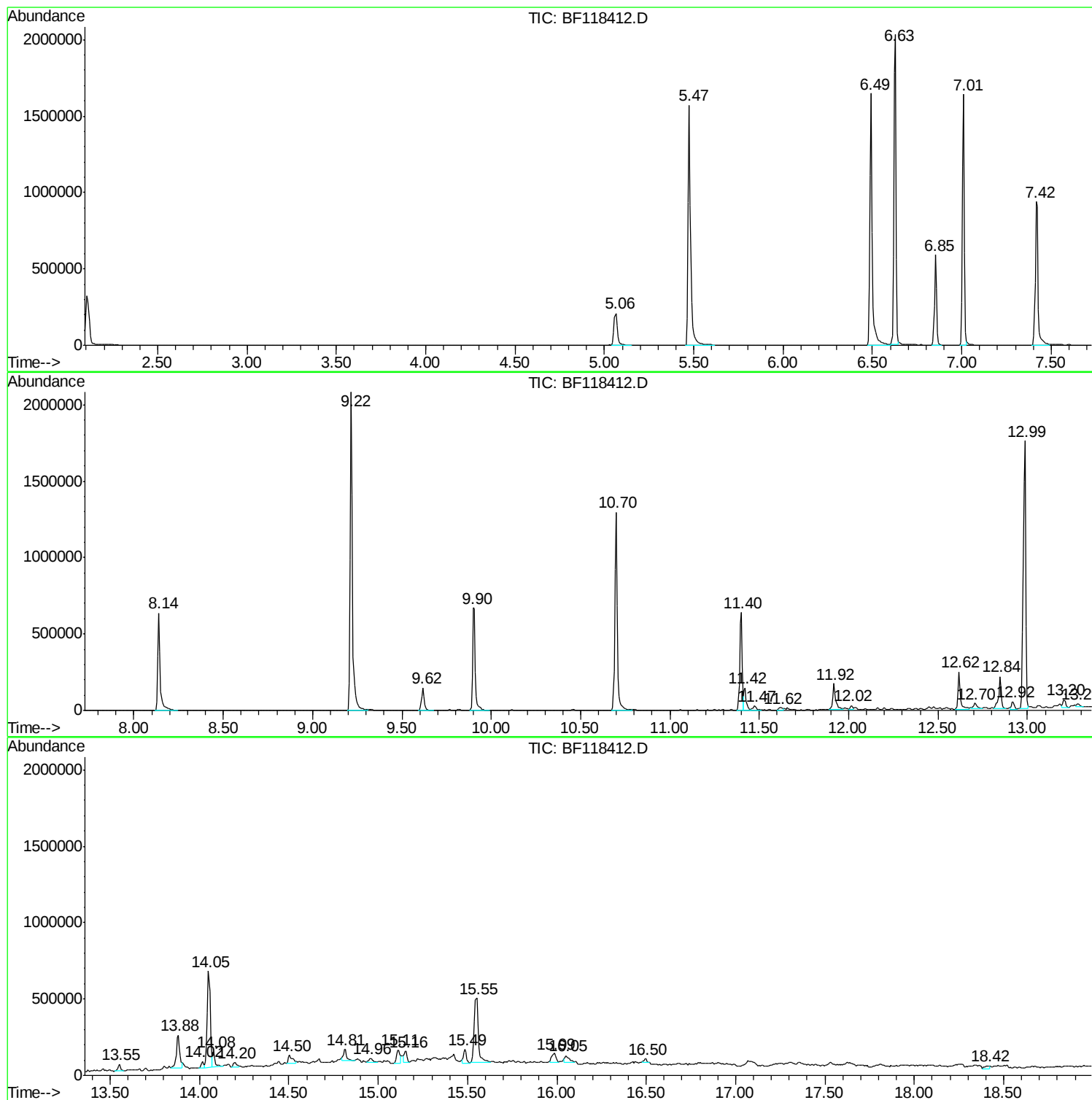
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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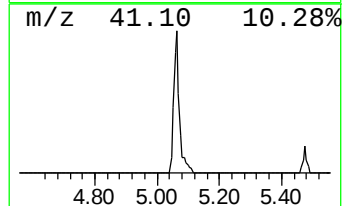
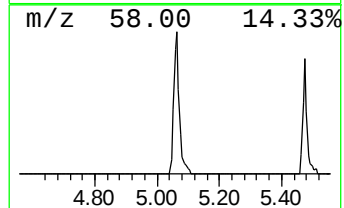
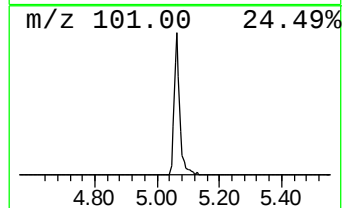
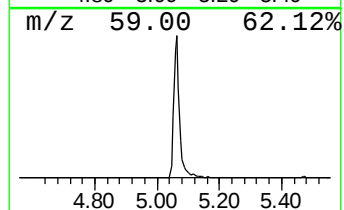
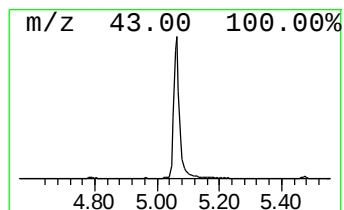
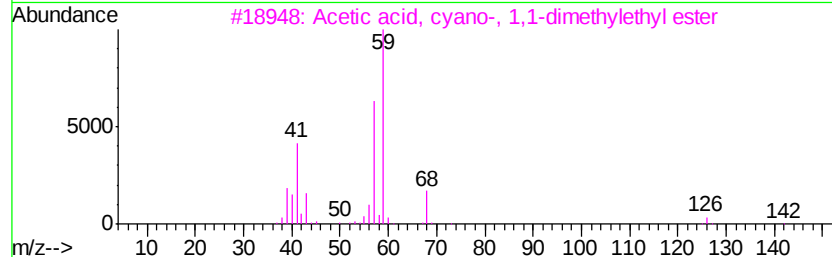
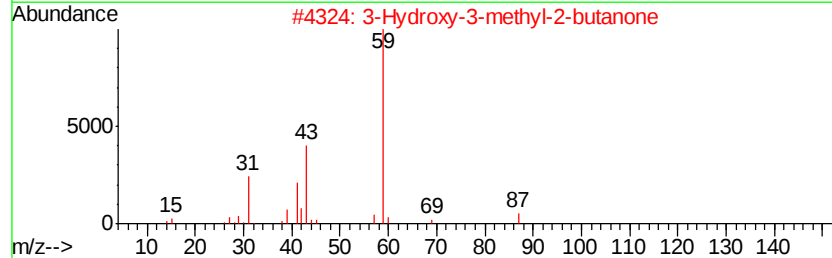
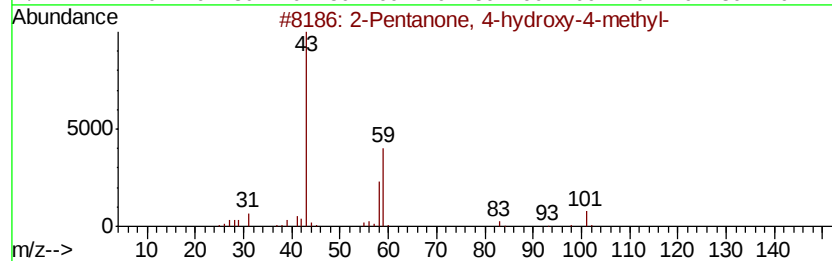
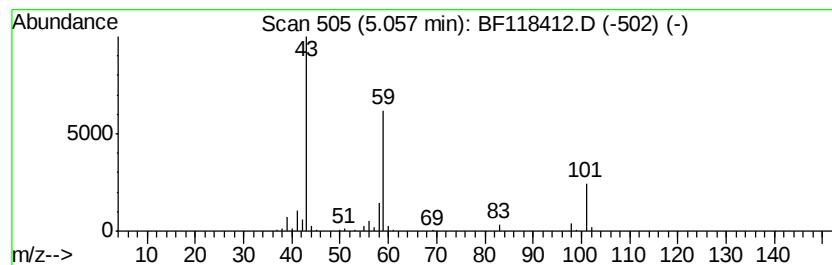
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	11.22 ng	265779	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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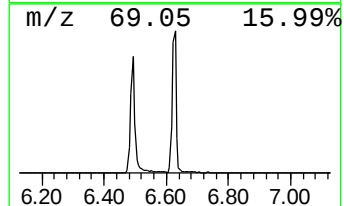
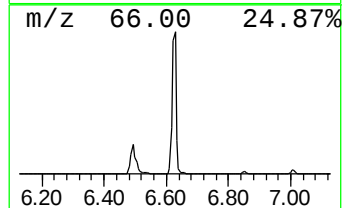
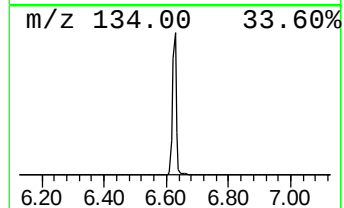
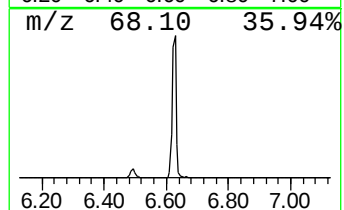
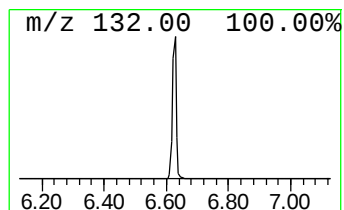
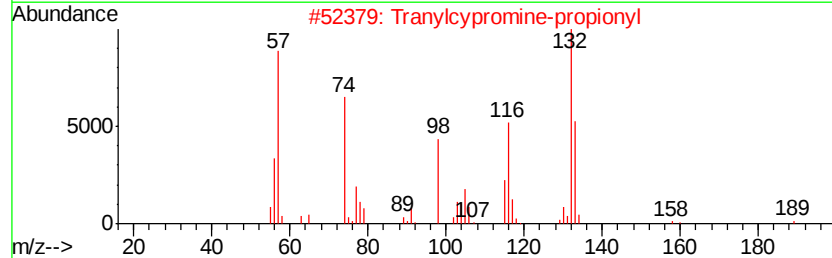
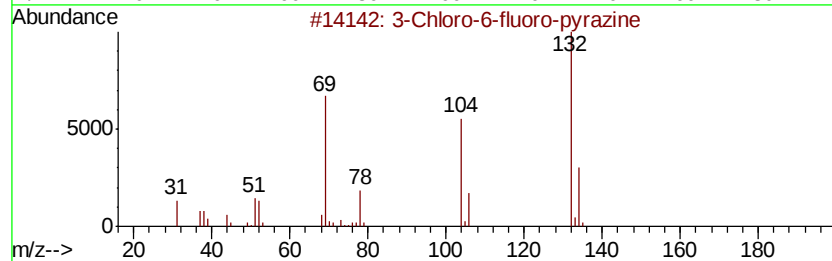
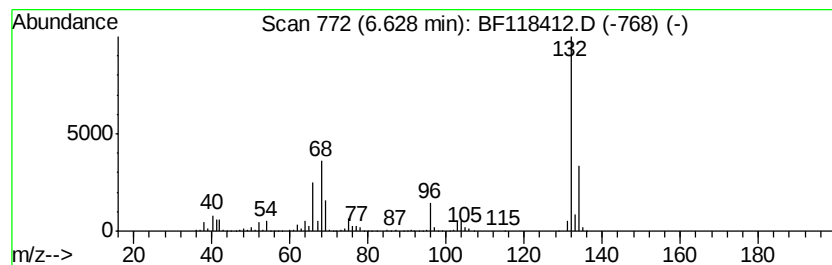
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	75.80 ng	1795540	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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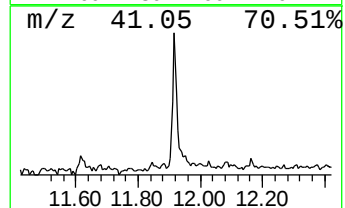
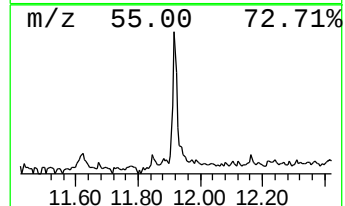
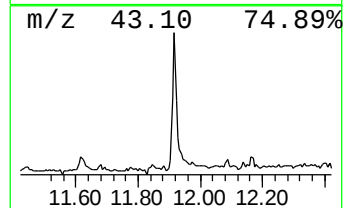
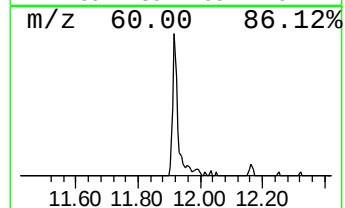
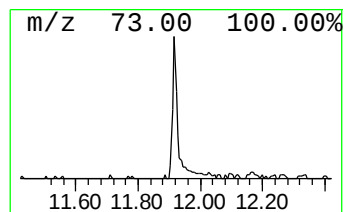
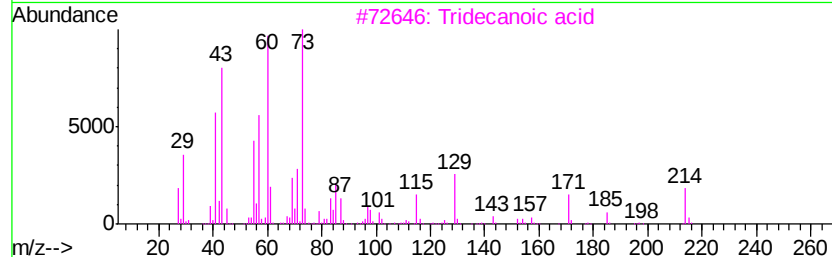
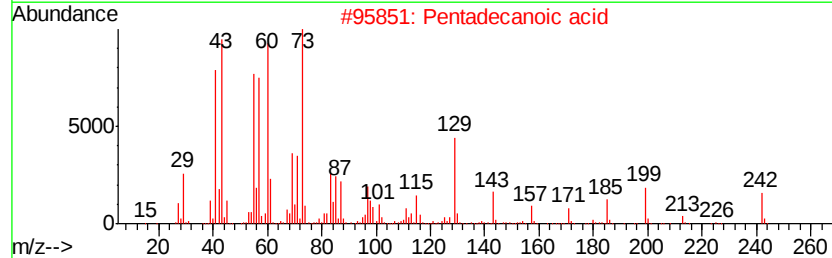
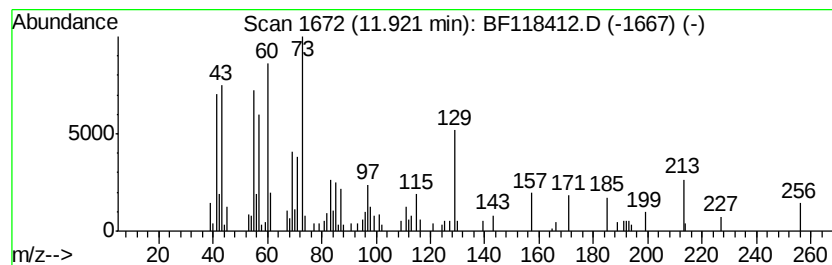
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	6.14 ng	189343	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	18
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	15



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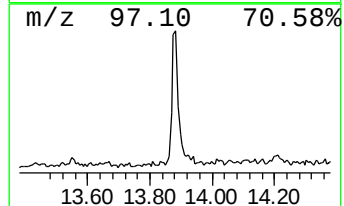
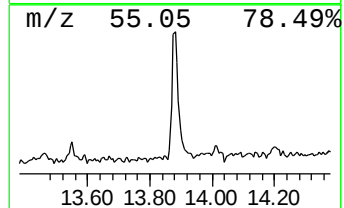
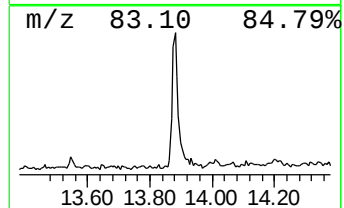
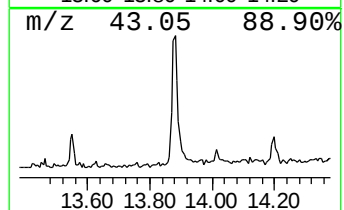
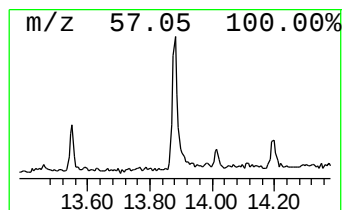
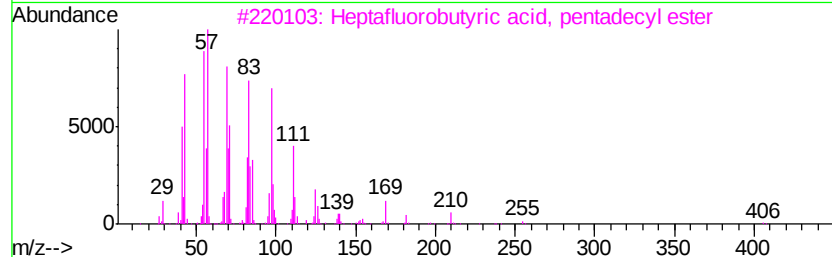
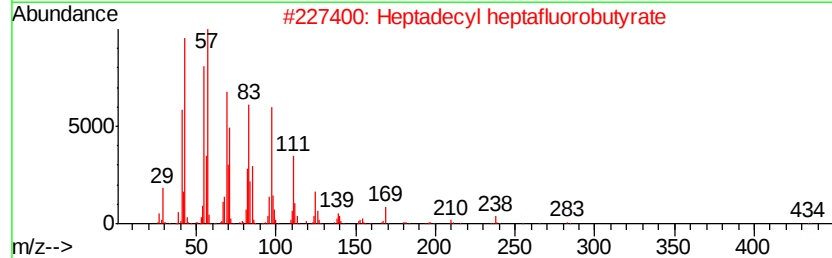
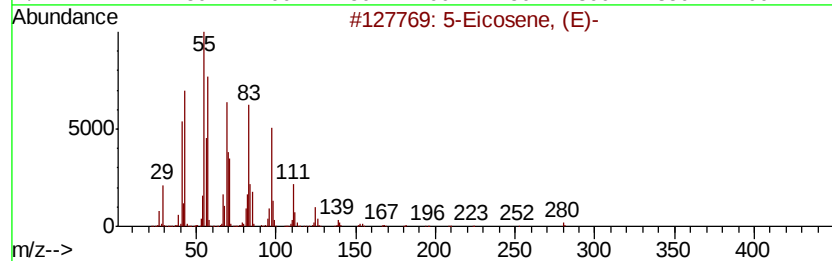
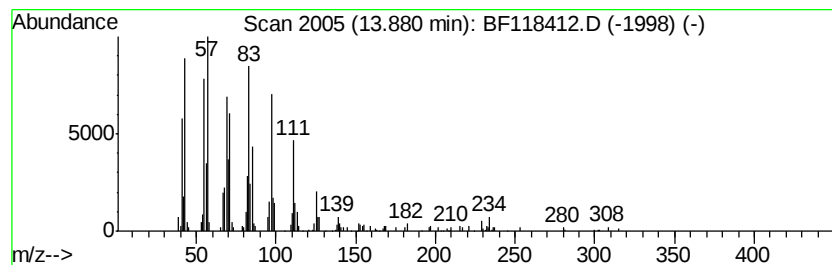
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Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.88	8.90 ng	301806	Chrysene-d12	14.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	96
2	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
3	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	91
4	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	91
5	Nonadecyl pentafluoropropionate		430	C22H39F5O2	1000351-88-8	91



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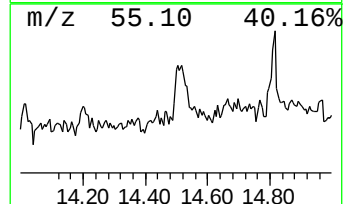
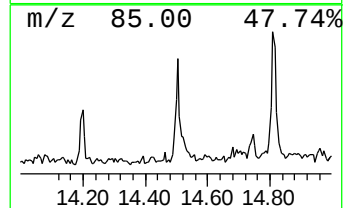
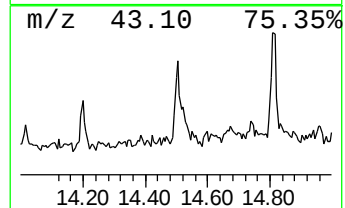
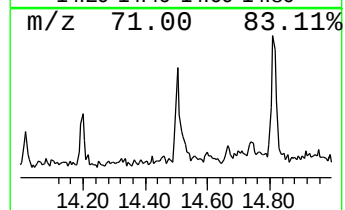
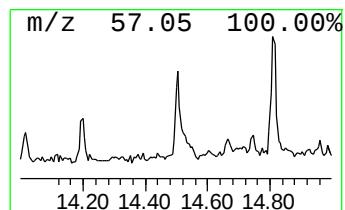
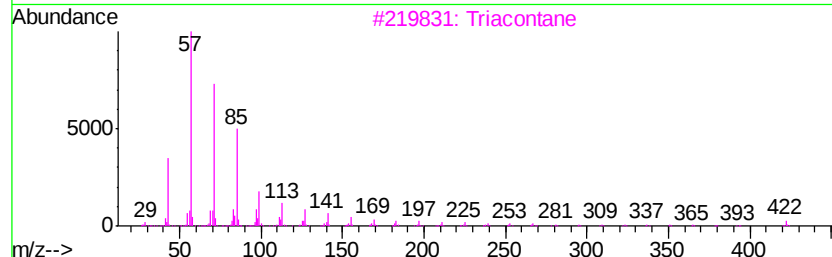
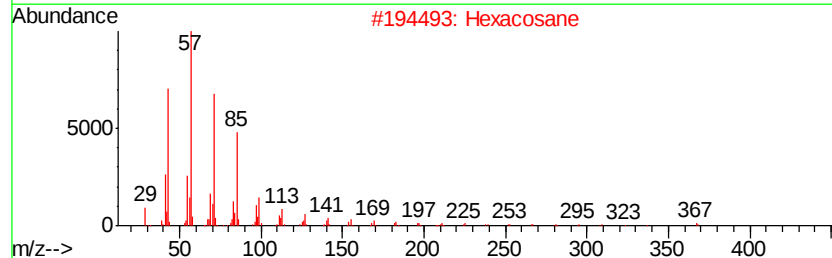
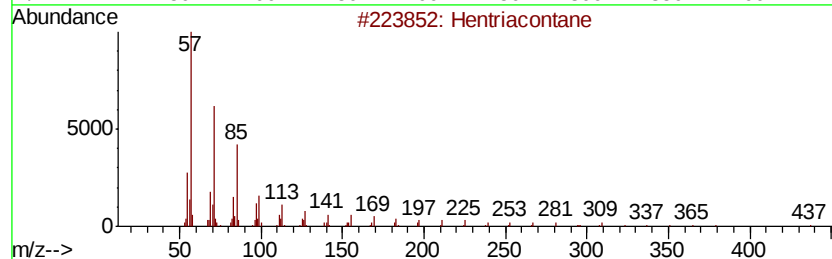
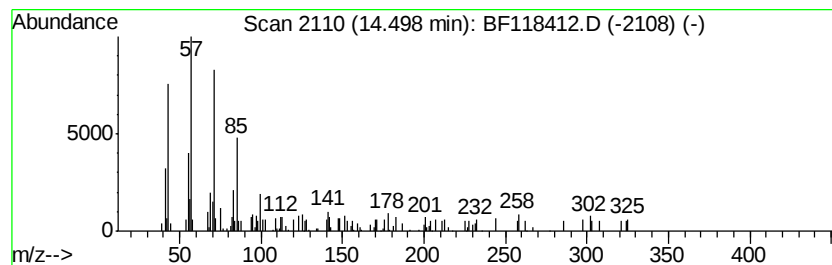
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Peak Number 6 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.81 ng	95301	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	68
2	Hexacosane		366	C26H54	000630-01-3	68
3	triacontane		422	C30H62	000638-68-6	64
4	Hexadecane		226	C16H34	000544-76-3	64
5	Tetracosane		338	C24H50	000646-31-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118412.D
Acq On : 31 Dec 2019 18:27
Operator : JU
Sample : K6465-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-9-(1-3)

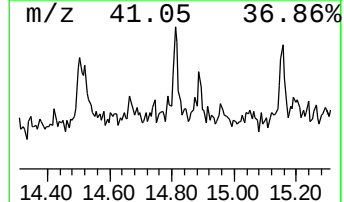
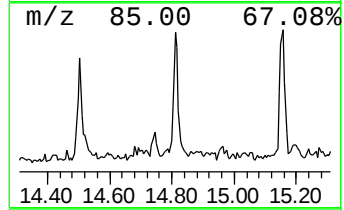
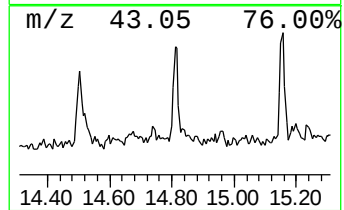
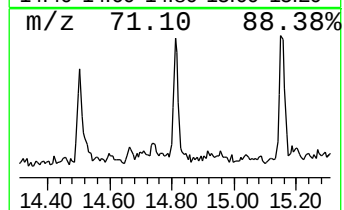
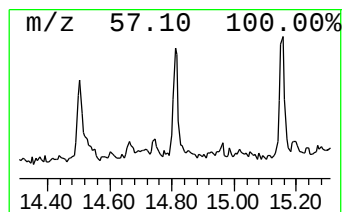
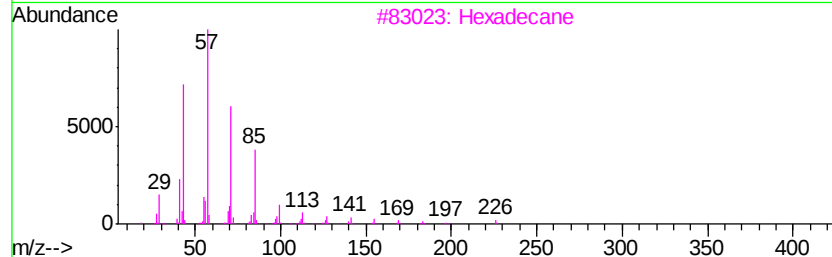
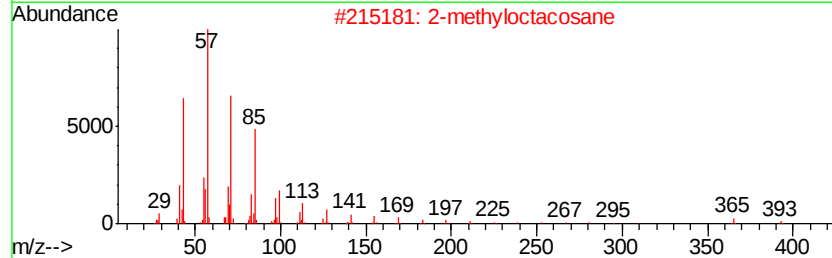
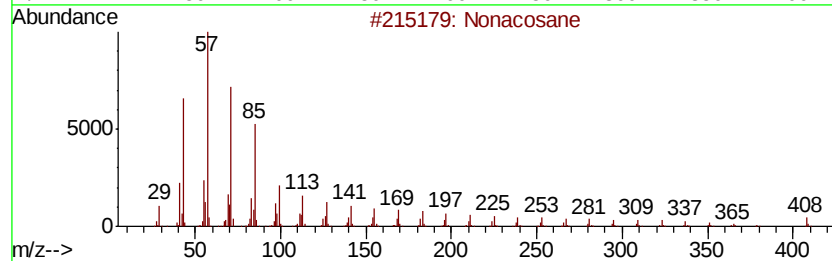
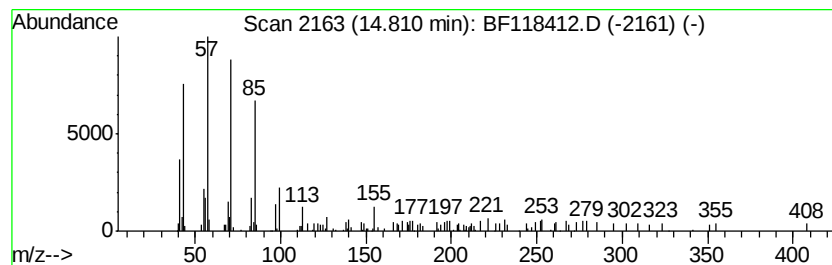
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.75 ng	89676	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonacosane	408	C29H60	000630-03-5	93
2		2-methyloctacosane	408	C29H60	1000376-72-8	72
3		Hexadecane	226	C16H34	000544-76-3	64
4		Hexacosane	366	C26H54	000630-01-3	64
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118412.D
Acq On : 31 Dec 2019 18:27
Operator : JU
Sample : K6465-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-9-(1-3)

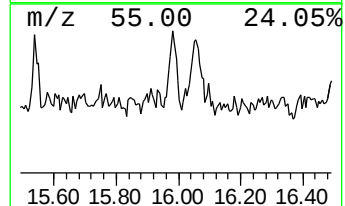
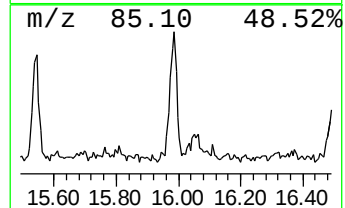
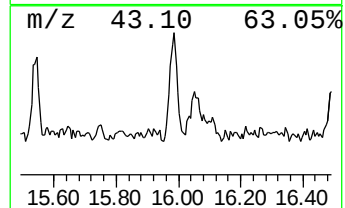
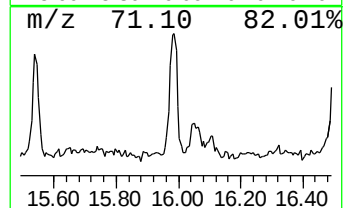
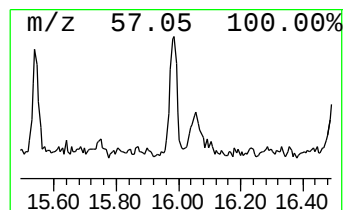
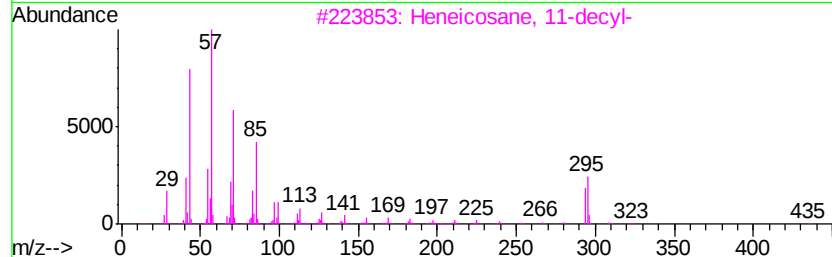
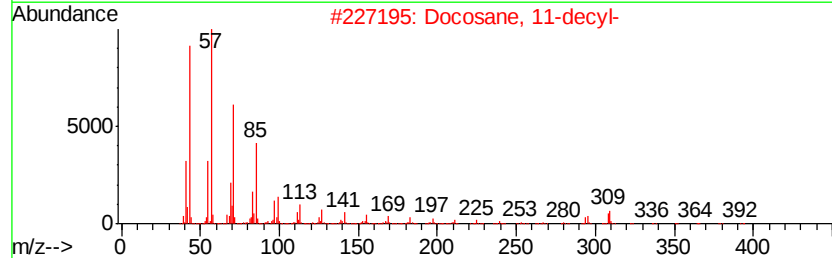
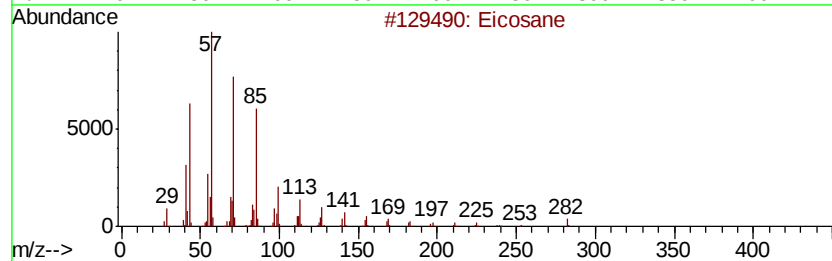
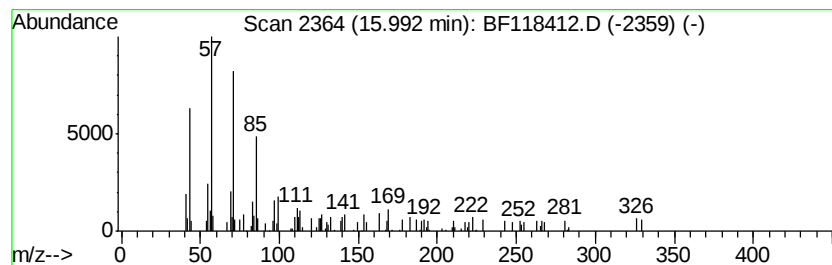
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.99	2.86 ng	93275	Perylene-d12	15.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	83
2	Docosane, 11-decyl-		451	C32H66	055401-55-3	62
3	Heneicosane, 11-decyl-		437	C31H64	055320-06-4	62
4	Eicosane, 10-hexyl-10-methyl-		380	C27H56	055282-32-1	58
5	Hexadecane		226	C16H34	000544-76-3	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123119\
Data File : BF118412.D
Acq On : 31 Dec 2019 18:27
Operator : JU
Sample : K6465-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-9-(1-3)

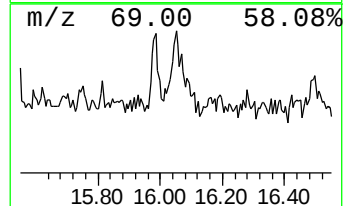
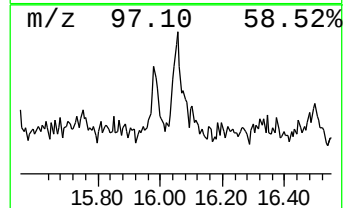
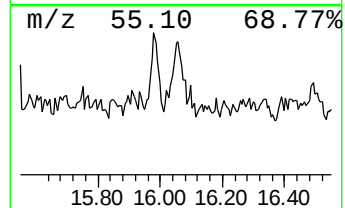
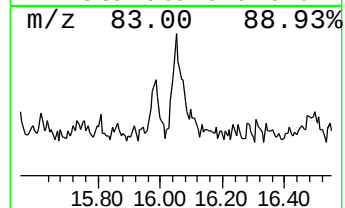
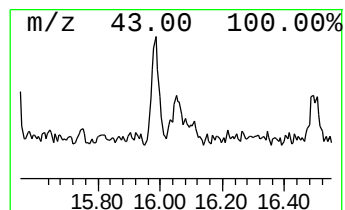
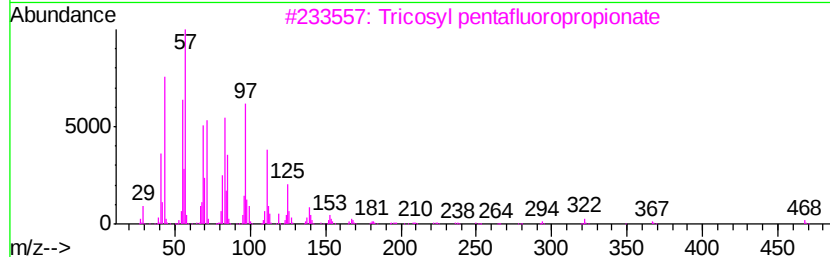
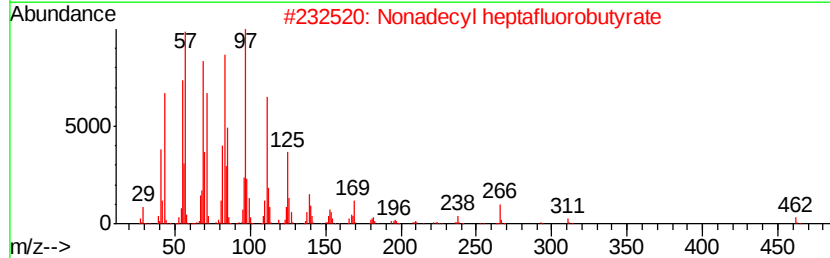
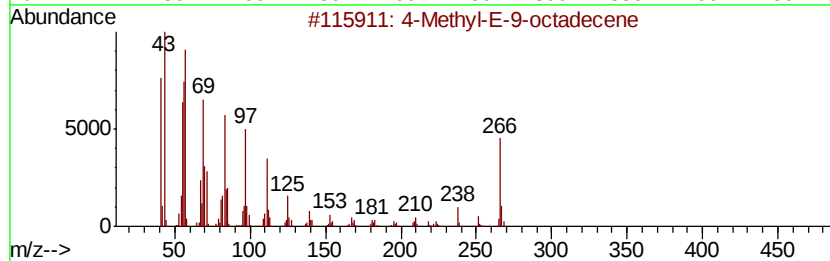
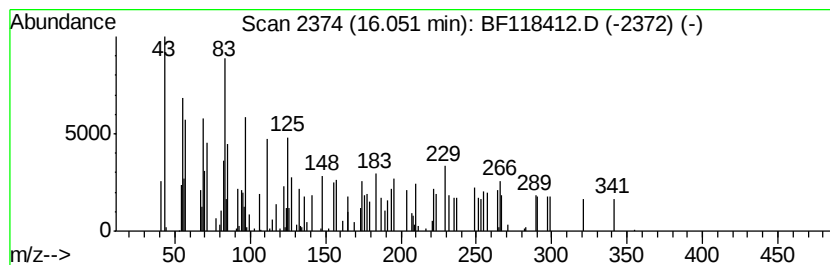
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.05 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.15 ng	70193	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	41
2		Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	30
3		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	27
4		Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	27
5		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF123119\
Data File : BF118412.D
Acq On : 31 Dec 2019 18:27
Operator : JU
Sample : K6465-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-9-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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
2-Pentanone, 4-hy...	5.06	11.2	ng	265779	1	6.85	473734	20.0
unknown6.63	6.63	75.8	ng	1795540	1	6.85	473734	20.0
n-Hexadecanoic acid	11.92	6.1	ng	189343	4	11.40	616960	20.0
5-Eicosene, (E)-	13.88	8.9	ng	301806	5	14.05	678355	20.0
Hentriacontane	14.50	2.8	ng	95301	5	14.05	678355	20.0
Nonacosane	14.81	2.8	ng	89676	6	15.55	652534	20.0
Eicosane	15.99	2.9	ng	93275	6	15.55	652534	20.0
unknown16.05	16.05	2.1	ng	70193	6	15.55	652534	20.0