

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
 Data File : BF118449.D
 Acq On : 2 Jan 2020 21:39
 Operator : JU
 Sample : K6465-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GP-4-(3-5)

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	5.051	500	504	513	rBV	238229	303062	12.23%	1.392%
2	5.463	571	574	600	rBV	1665598	1767760	71.34%	8.118%
3	6.487	744	748	766	rBV	2200832	2125481	85.78%	9.761%
4	6.616	766	770	774	rBV	2416793	2260439	91.23%	10.381%
5	6.845	805	809	818	rVB	701666	565230	22.81%	2.596%
6	7.004	832	836	848	rBV	1878303	1733153	69.95%	7.959%
7	7.416	901	906	923	rBV	1177430	1220184	49.24%	5.603%
8	8.134	1024	1028	1045	rBV	731194	737941	29.78%	3.389%
9	9.210	1207	1211	1214	rBV	3130942	2477869	100.00%	11.379%
10	9.610	1275	1279	1287	rBV	103126	103060	4.16%	0.473%
11	9.892	1324	1327	1343	rVB	961999	824106	33.26%	3.785%
12	10.686	1458	1462	1477	rBV	1448042	1502307	60.63%	6.899%
13	11.386	1578	1581	1584	rBV	866177	782491	31.58%	3.593%
14	11.410	1584	1585	1590	rVB	106406	82784	3.34%	0.380%
15	11.616	1616	1620	1622	rBV3	21362	29863	1.21%	0.137%
16	11.910	1665	1670	1678	rBV3	184230	224099	9.04%	1.029%
17	12.610	1785	1789	1794	rBV	152768	148825	6.01%	0.683%
18	12.698	1801	1804	1811	rBV2	31719	37521	1.51%	0.172%
19	12.839	1823	1828	1831	rBV	137910	139590	5.63%	0.641%
20	12.974	1847	1851	1855	rBV	2328376	2148212	86.70%	9.865%
21	13.539	1943	1947	1949	rBV2	43673	40642	1.64%	0.187%
22	13.868	2000	2003	2016	rVB4	148020	275141	11.10%	1.264%
23	14.039	2028	2032	2036	rBV	628576	685237	27.65%	3.147%
24	14.068	2036	2037	2040	rVB	67175	36007	1.45%	0.165%
25	14.186	2054	2057	2059	rBV	76816	64973	2.62%	0.298%
26	14.492	2106	2109	2111	rBV	94347	89792	3.62%	0.412%
27	14.798	2157	2161	2165	rVB	99191	100377	4.05%	0.461%
28	14.874	2170	2174	2177	rBV	110148	106979	4.32%	0.491%
29	15.092	2208	2211	2214	rBV	48055	67943	2.74%	0.312%
30	15.133	2214	2218	2225	rVB2	99285	139116	5.61%	0.639%
31	15.398	2260	2263	2271	rVB	30414	41978	1.69%	0.193%
32	15.468	2271	2275	2279	rBV	43501	50335	2.03%	0.231%
33	15.527	2279	2285	2297	rVB	489471	693449	27.99%	3.185%
34	15.957	2353	2358	2363	rBV	55397	89630	3.62%	0.412%

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GP-4-(3-5)

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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35	16.039	2366	2372	2374	rBV6	18602	34156	1.38%	0.157%
36	16.468	2441	2445	2451	rVB4	28185	45902	1.85%	0.211%

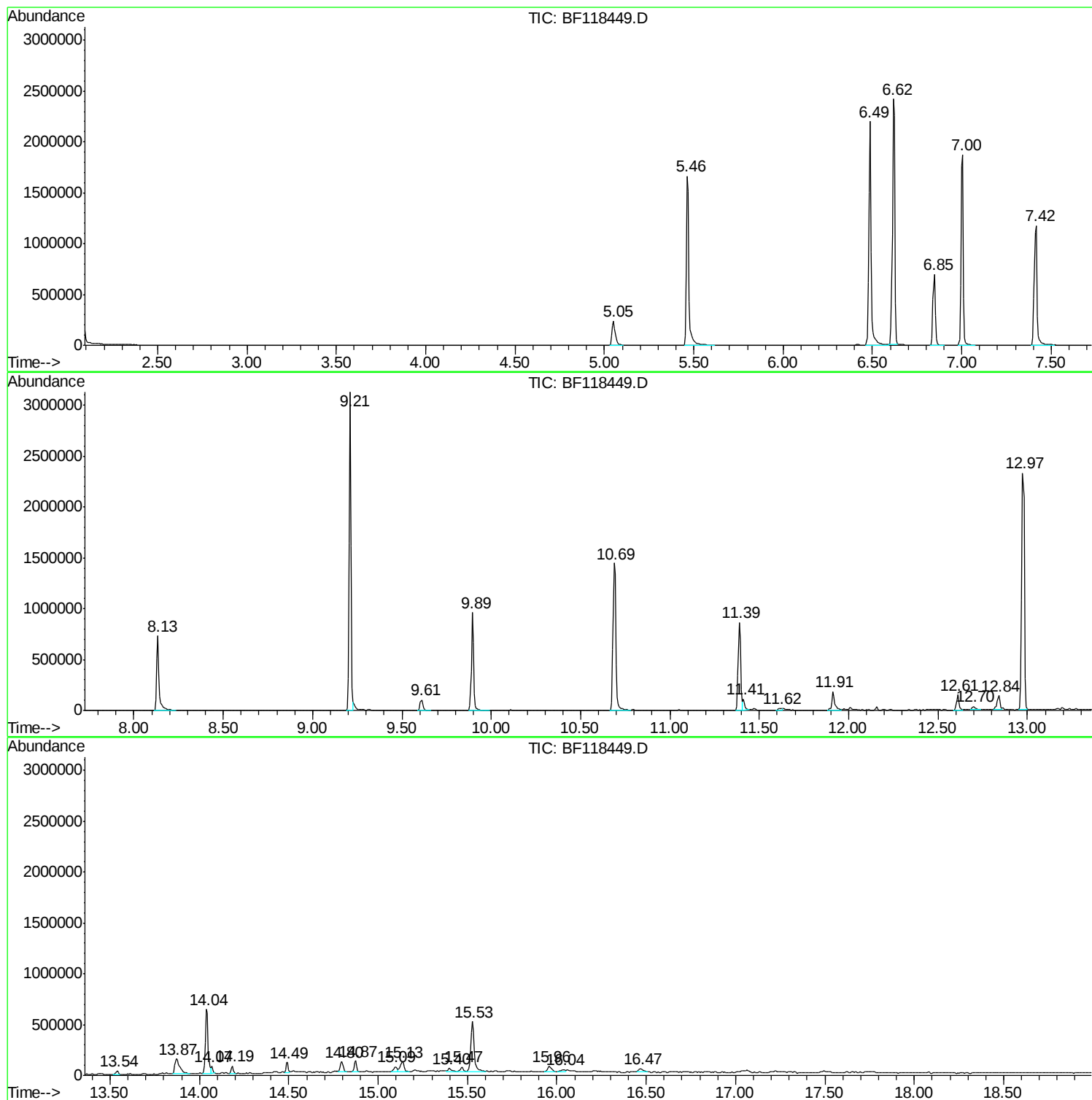
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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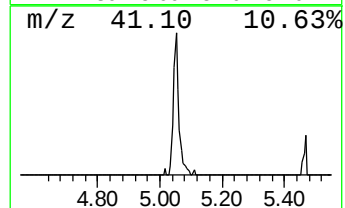
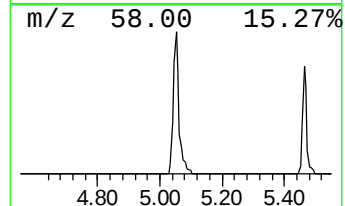
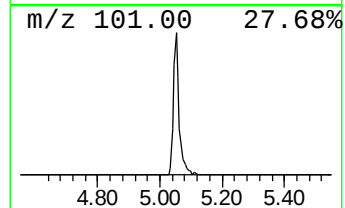
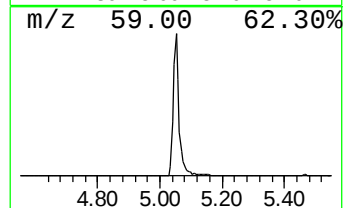
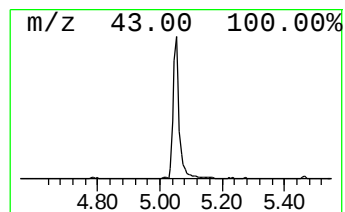
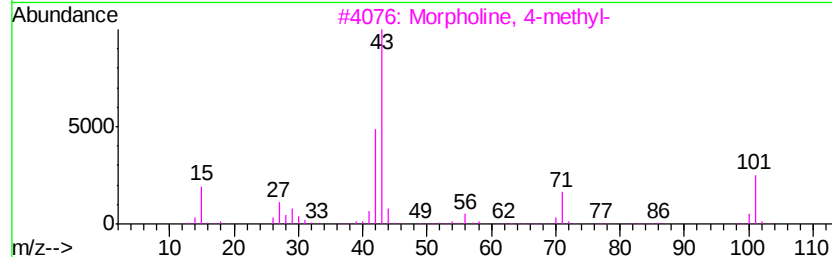
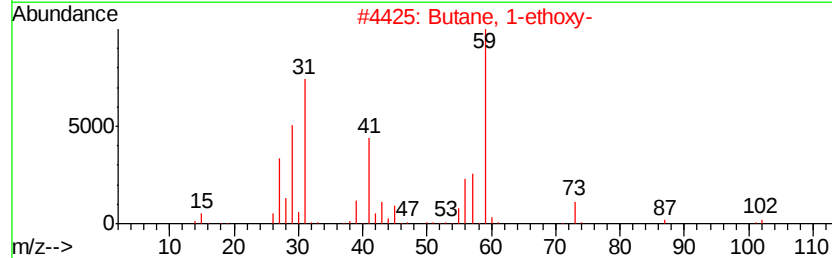
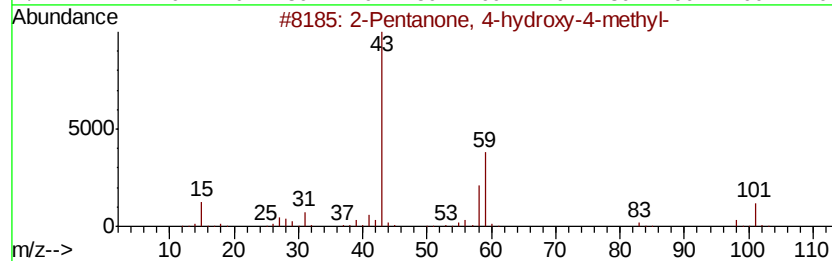
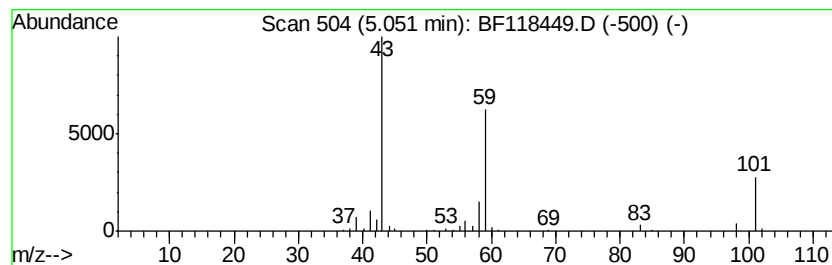
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	10.72 ng	303062	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Silane, trimethyl-	74	C3H10Si	000993-07-7	9



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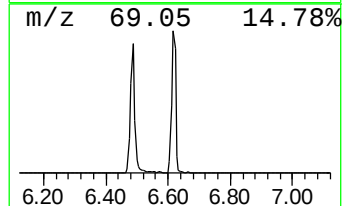
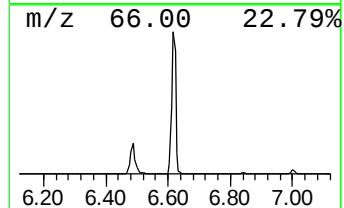
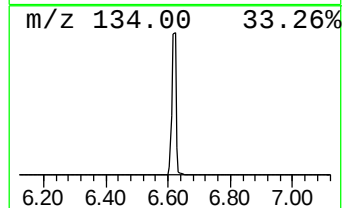
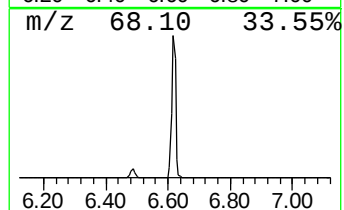
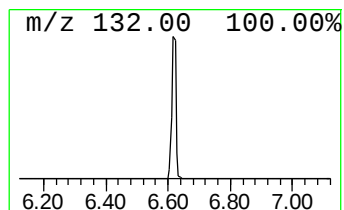
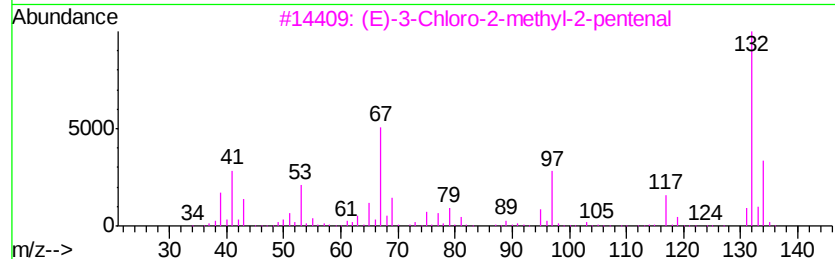
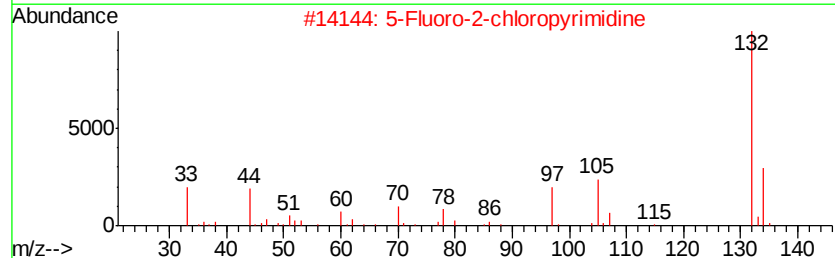
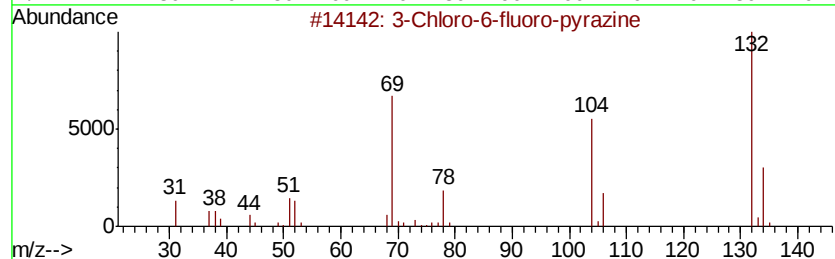
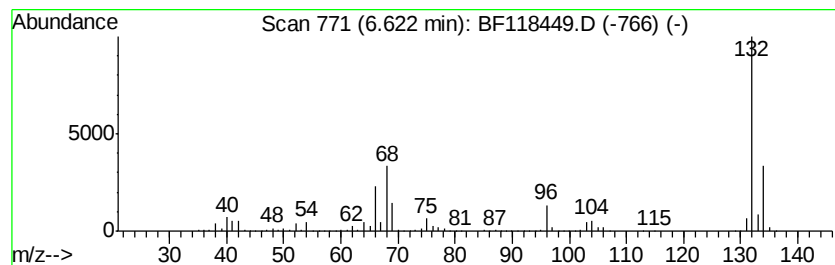
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	79.98 ng	2260440	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	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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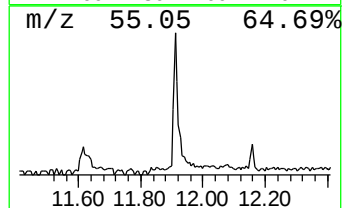
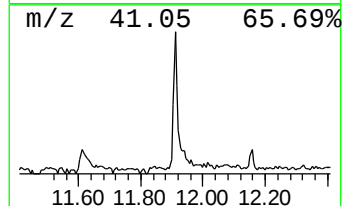
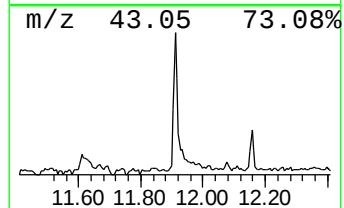
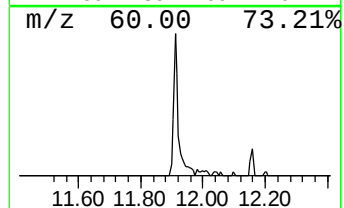
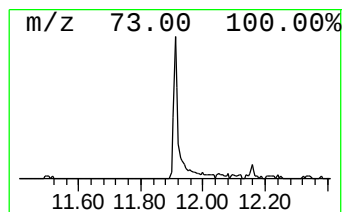
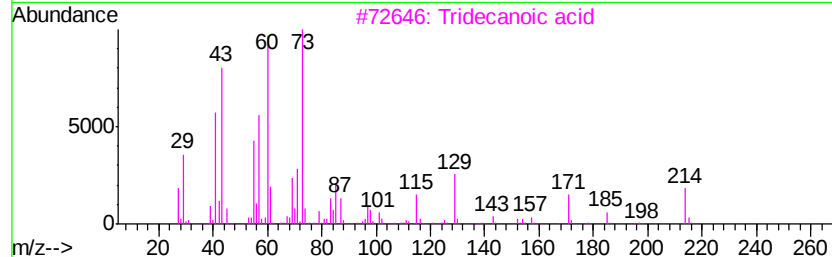
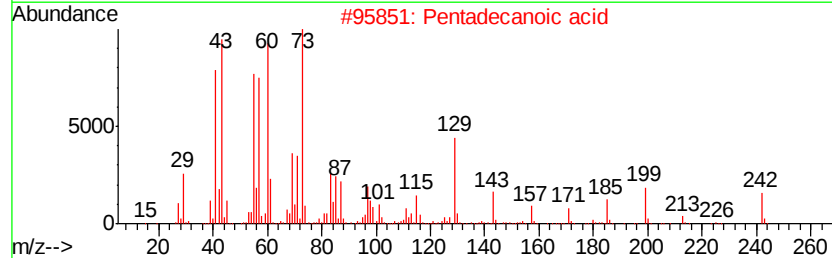
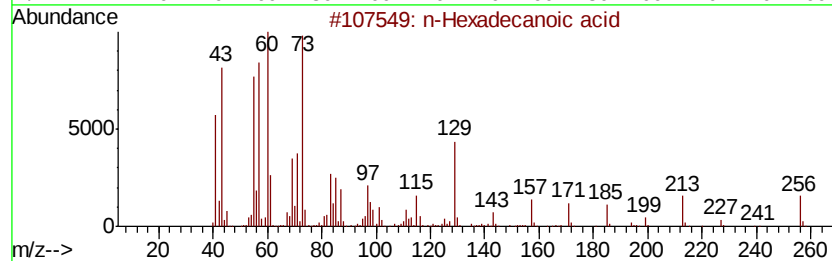
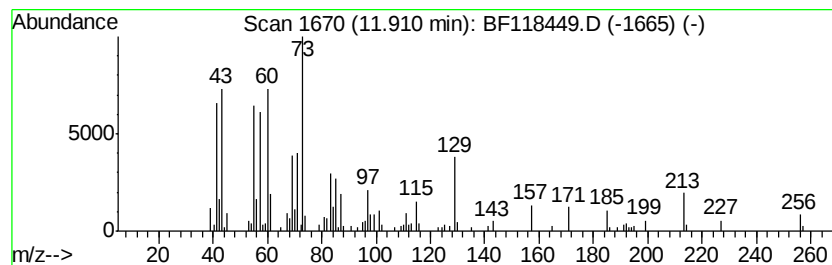
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	5.73 ng	224099	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	20
5	Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	18



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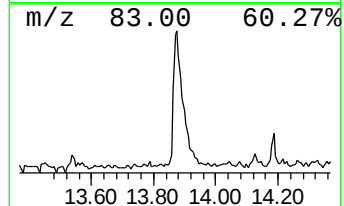
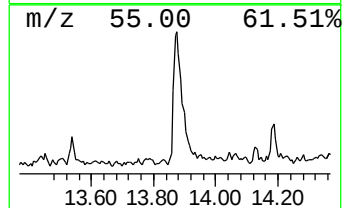
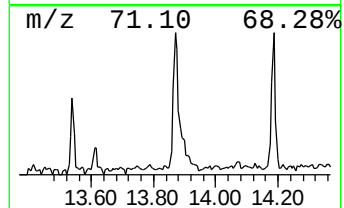
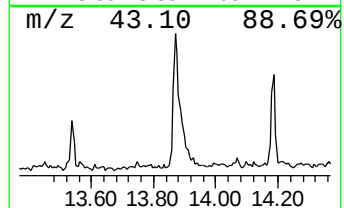
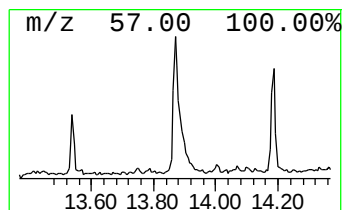
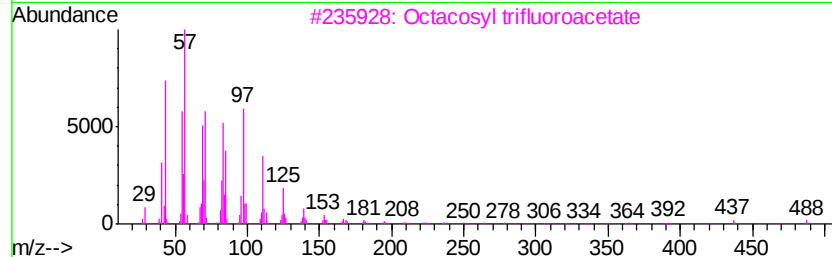
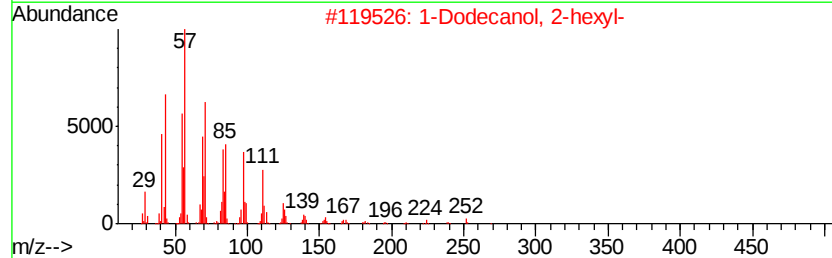
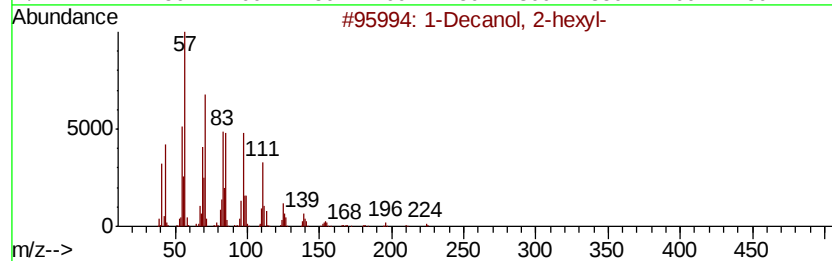
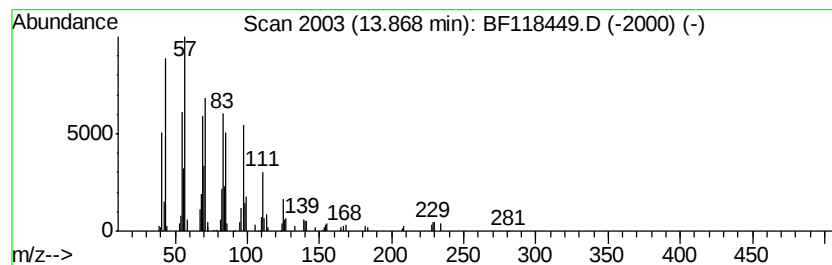
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Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.03 ng	275141	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
3		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	81
4		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	81
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	68



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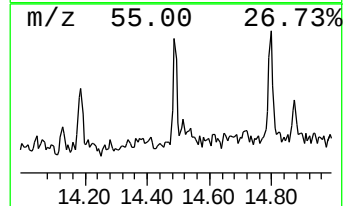
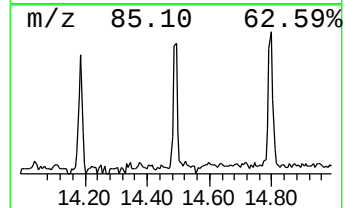
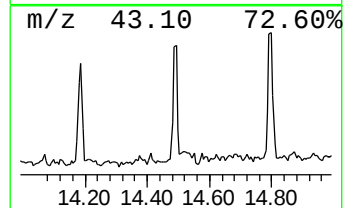
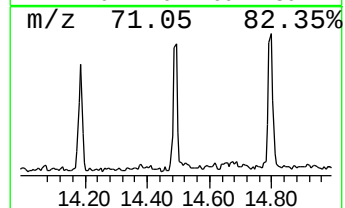
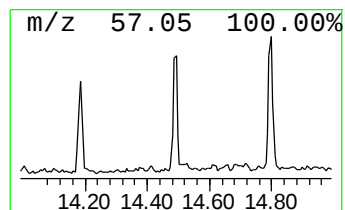
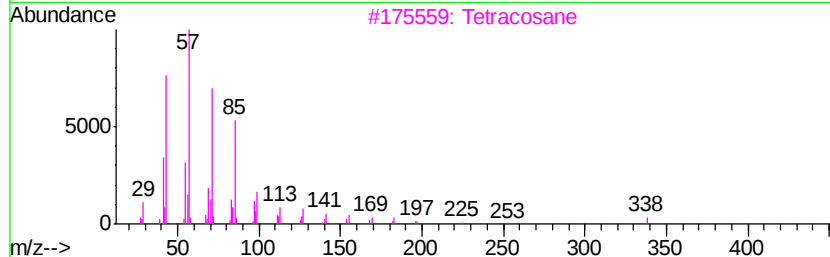
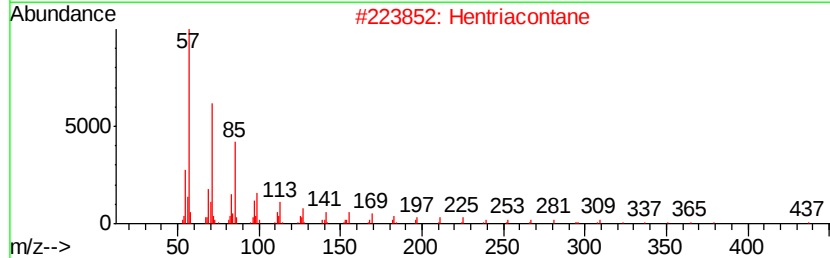
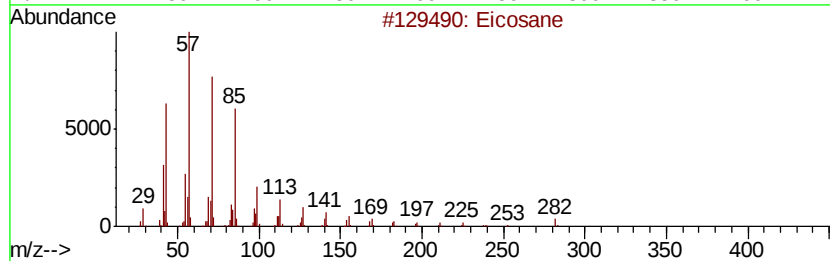
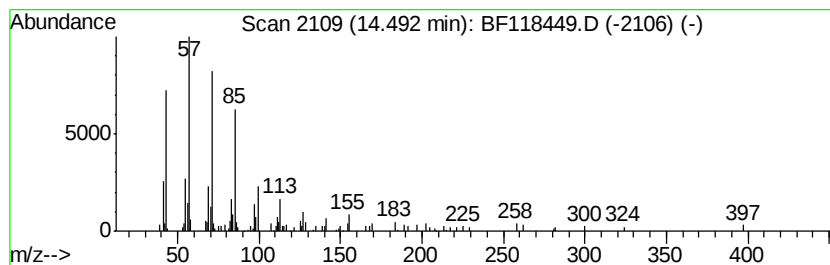
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Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.62 ng	89792	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Hentriacontane		437	C31H64	000630-04-6	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118449.D
Acq On : 2 Jan 2020 21:39
Operator : JU
Sample : K6465-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

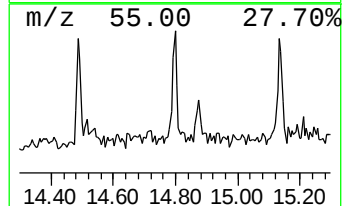
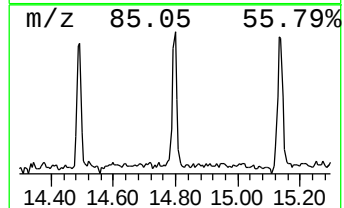
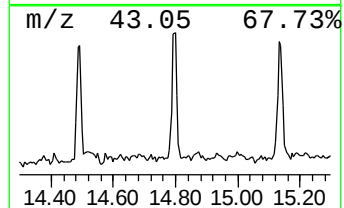
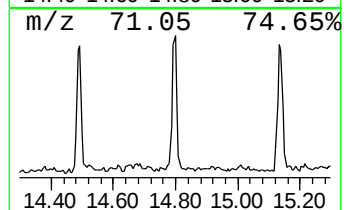
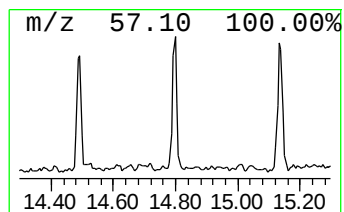
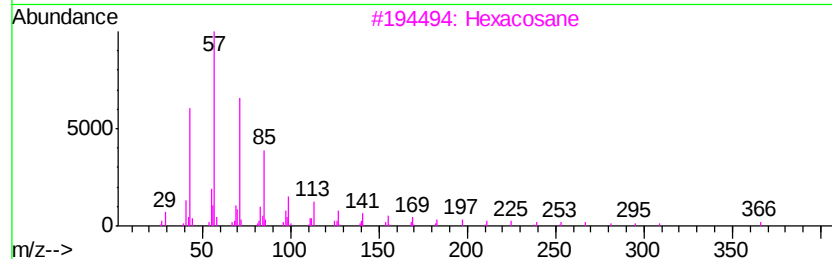
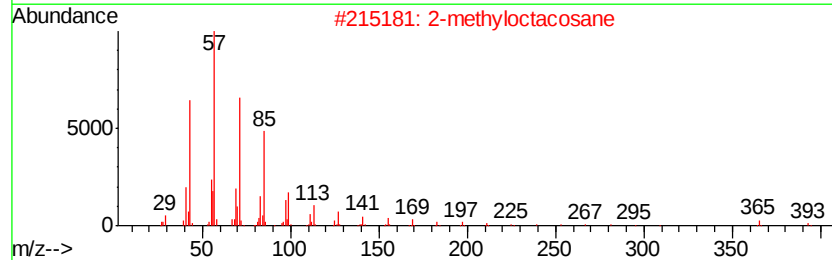
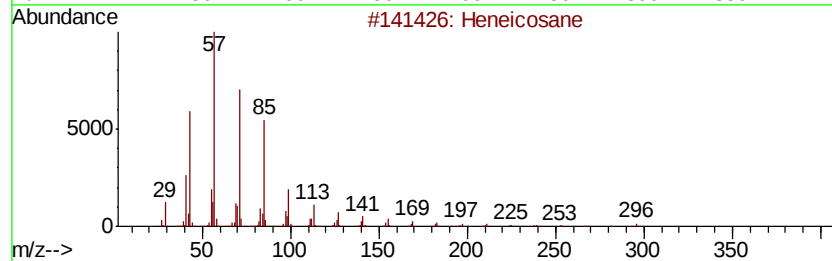
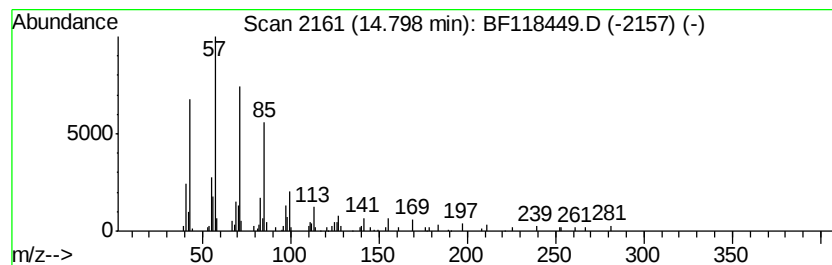
Instrument :
BNA_F
ClientSampleId :
GP-4-(3-5)

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 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	2.90 ng	100377	Perylene-d12	15.53
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	Hexacosane	366 C26H54	000630-01-3	91
4	triacontane	422 C30H62	000638-68-6	91
5	Pentacosane	352 C25H52	000629-99-2	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
 Data File : BF118449.D
 Acq On : 2 Jan 2020 21:39
 Operator : JU
 Sample : K6465-08
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

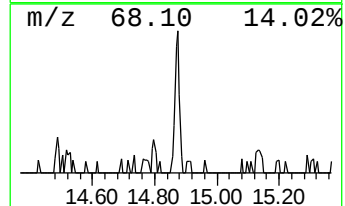
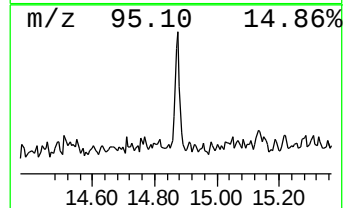
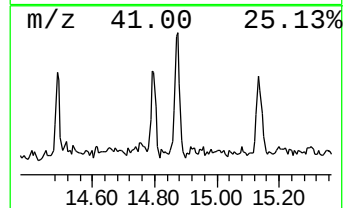
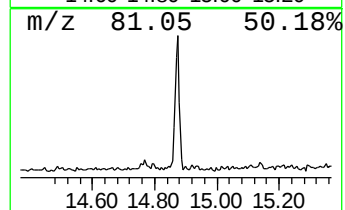
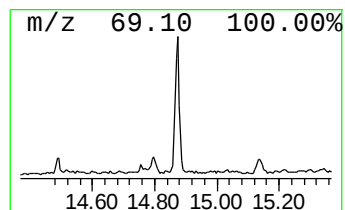
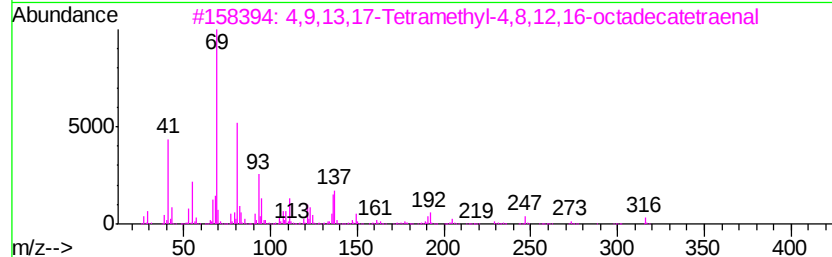
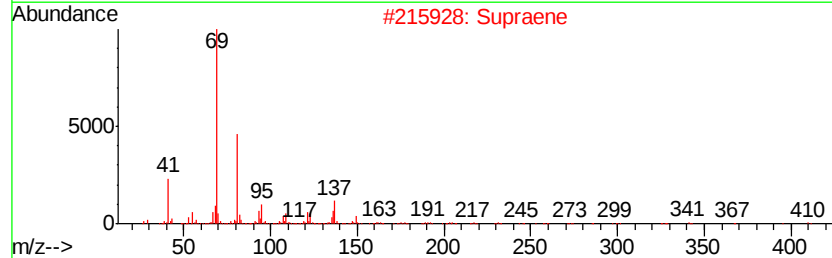
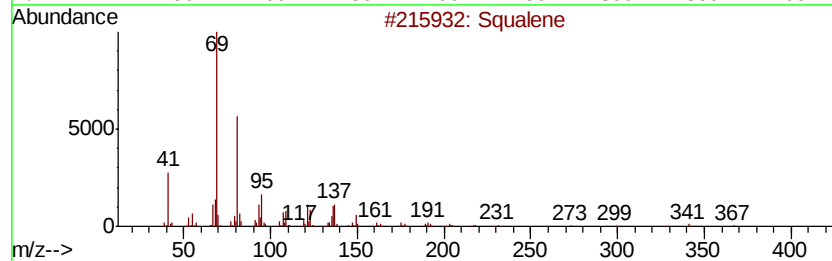
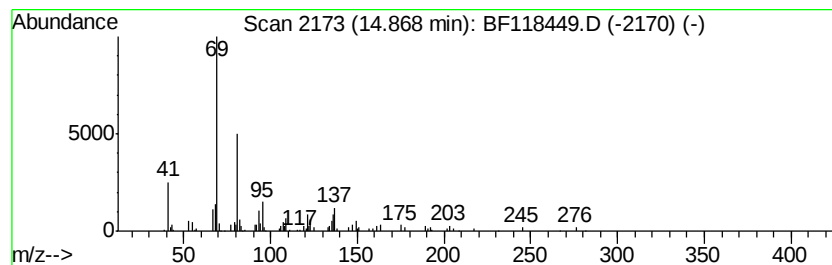
Instrument :
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 ClientSampleId :
 GP-4-(3-5)

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 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.87	3.09 ng	106979	Perylene-d12		15.53		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	90
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
5			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118449.D
Acq On : 2 Jan 2020 21:39
Operator : JU
Sample : K6465-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-4-(3-5)

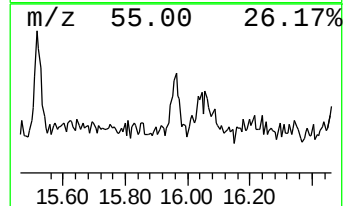
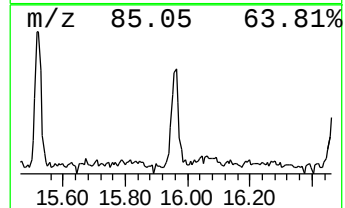
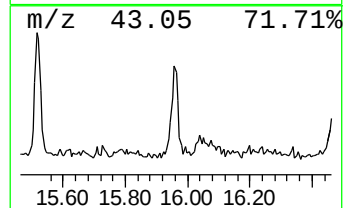
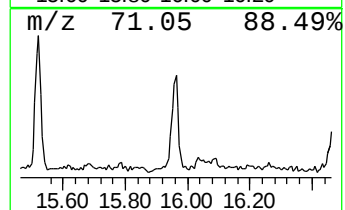
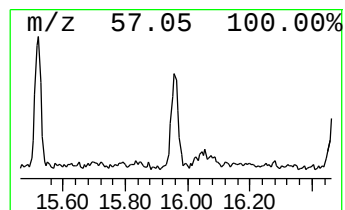
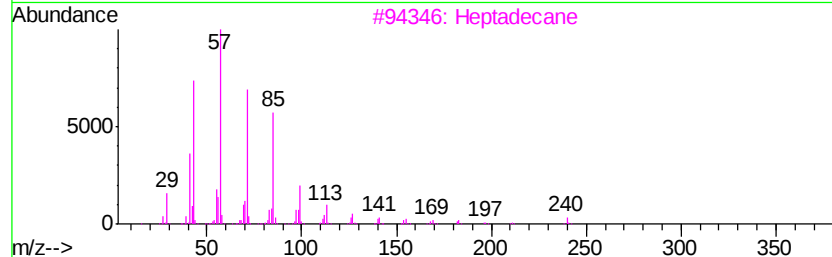
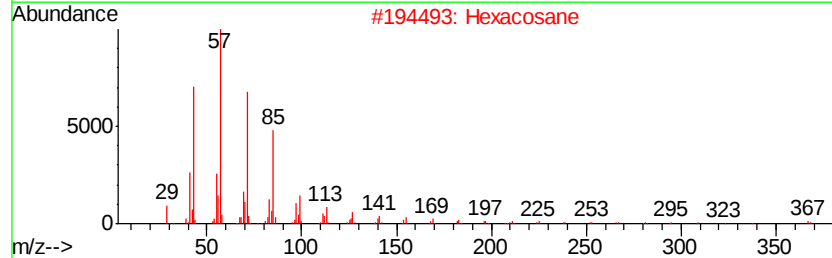
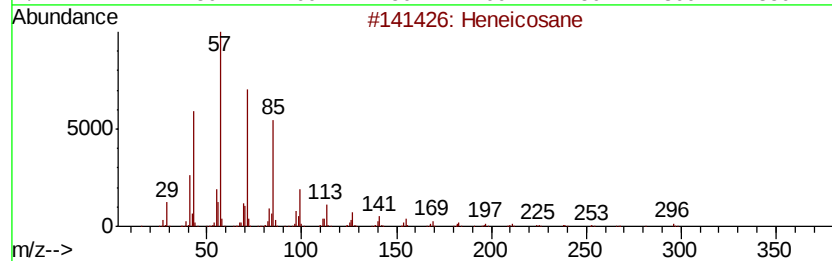
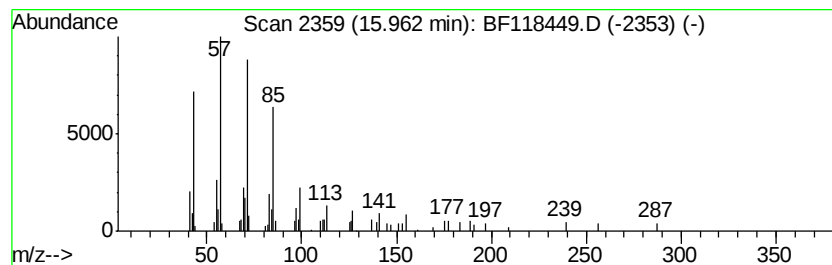
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	2.59 ng	89630	Perylene-d12	15.53

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Hexacosane		366	C26H54	000630-01-3	87
3	Heptadecane		240	C17H36	000629-78-7	87
4	Octacosane		394	C28H58	000630-02-4	86
5	2-methyloctacosane		408	C29H60	1000376-72-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010220\
Data File : BF118449.D
Acq On : 2 Jan 2020 21:39
Operator : JU
Sample : K6465-08
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-4-(3-5)

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...	5.05	10.7	ng	303062	1	6.85	565230	20.0
unknown6.62	6.62	80.0	ng	2260440	1	6.85	565230	20.0
n-Hexadecanoic acid	11.91	5.7	ng	224099	4	11.39	782491	20.0
1-Decanol, 2-hexyl-	13.87	8.0	ng	275141	5	14.04	685237	20.0
Eicosane	14.49	2.6	ng	89792	5	14.04	685237	20.0
Heneicosane	14.80	2.9	ng	100377	6	15.53	693449	20.0
Squalene	14.87	3.1	ng	106979	6	15.53	693449	20.0
2-methyloctacosane	15.96	2.6	ng	89630	6	15.53	693449	20.0