

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
 Data File : BF114391.D
 Acq On : 18 May 2019 15:18
 Operator : JU/SJ
 Sample : K2905-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GIS-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-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	2.122	3	6	29	rVB	1132396	1514036	30.33%	2.998%
2	5.469	571	575	599	rBV	4443561	4649883	93.14%	9.208%
3	6.481	743	747	765	rBV	4683613	4928024	98.71%	9.758%
4	6.610	765	769	783	rVB	5043555	4702962	94.20%	9.313%
5	6.834	804	807	817	rBV	1554825	1334074	26.72%	2.642%
6	6.992	830	834	849	rBV	3880186	3514788	70.40%	6.960%
7	7.398	898	903	916	rBV	3129371	3103175	62.16%	6.145%
8	8.116	1021	1025	1043	rBV	1761570	1735100	34.75%	3.436%
9	9.186	1203	1207	1218	rBV	5216429	4751015	95.16%	9.408%
10	9.581	1270	1274	1286	rBV	720741	697917	13.98%	1.382%
11	9.869	1319	1323	1332	rVB	1950637	1883204	37.72%	3.729%
12	10.657	1453	1457	1472	rBV	3241683	3190932	63.91%	6.319%
13	11.351	1571	1575	1585	rBV	2132427	2070543	41.47%	4.100%
14	11.874	1661	1664	1674	rBV2	258810	340484	6.82%	0.674%
15	12.657	1794	1797	1806	rBV	61351	91576	1.83%	0.181%
16	12.933	1839	1844	1852	rBV	5193872	4992614	100.00%	9.886%
17	13.157	1876	1882	1890	rBV3	32618	66385	1.33%	0.131%
18	13.821	1991	1995	2012	rBV	646856	1080330	21.64%	2.139%
19	13.992	2020	2024	2033	rVB	1703121	1733658	34.72%	3.433%
20	14.145	2047	2050	2057	rBV	98496	101122	2.03%	0.200%
21	14.451	2099	2102	2111	rBV	168567	214293	4.29%	0.424%
22	14.757	2151	2154	2163	rBV	249549	254683	5.10%	0.504%
23	14.833	2163	2167	2171	rVB	152007	145041	2.91%	0.287%
24	15.092	2207	2211	2216	rBV	316628	339357	6.80%	0.672%
25	15.468	2269	2275	2285	rBV	1449101	2035352	40.77%	4.030%
26	15.892	2342	2347	2354	rBV	311733	467750	9.37%	0.926%
27	15.968	2355	2360	2365	rBV8	39324	97027	1.94%	0.192%
28	16.392	2426	2432	2445	rVB2	170111	353503	7.08%	0.700%
29	16.968	2526	2530	2538	rVB2	54859	111104	2.23%	0.220%

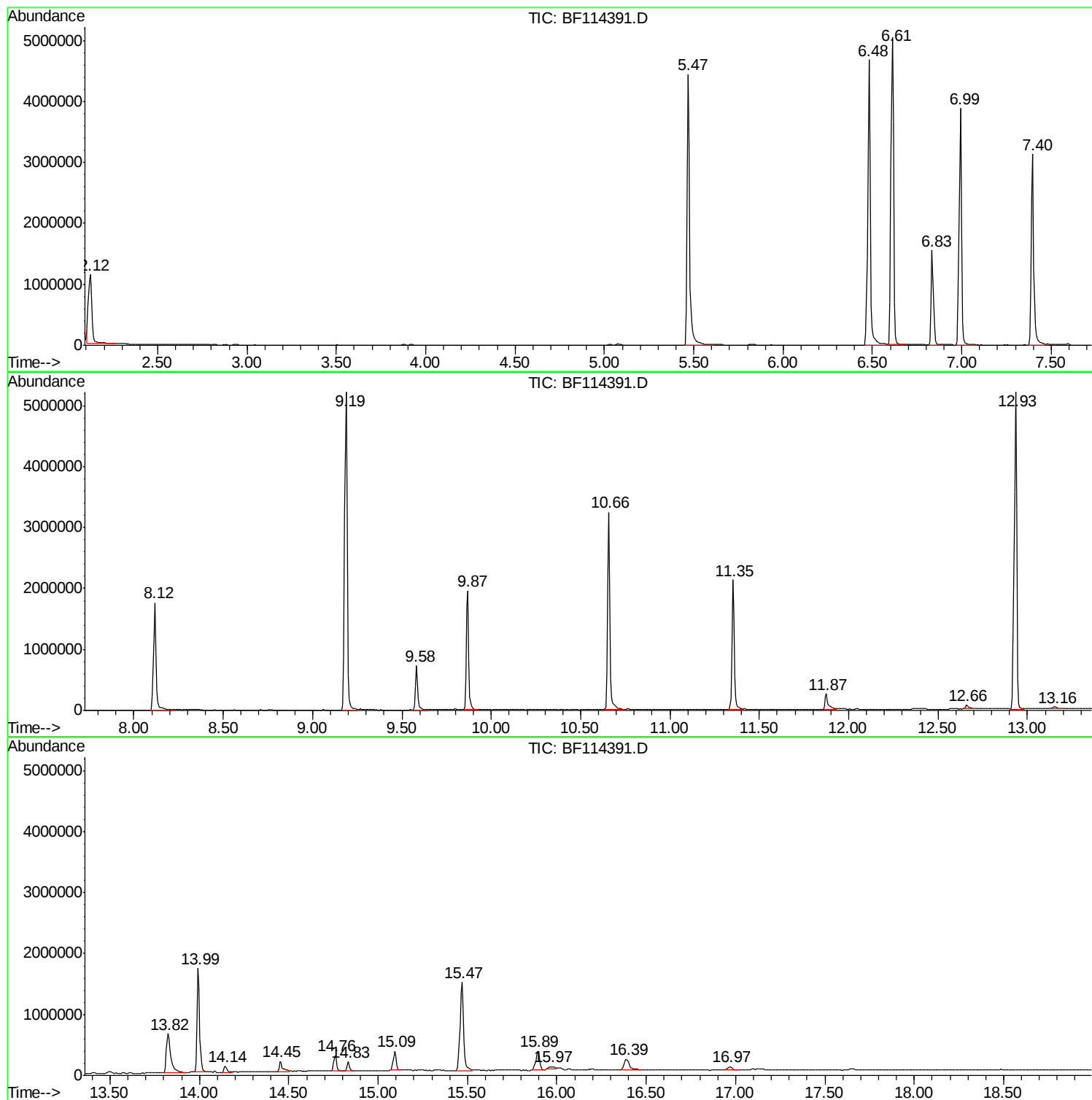
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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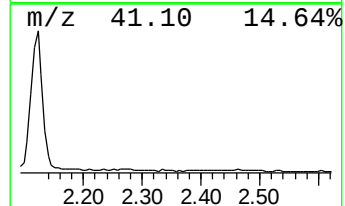
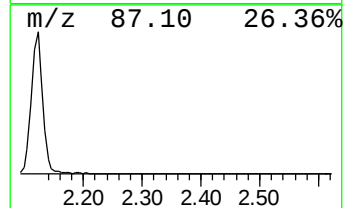
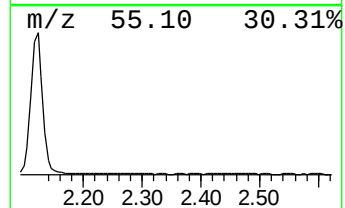
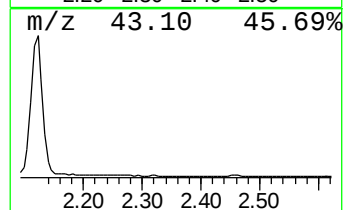
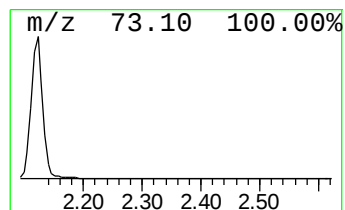
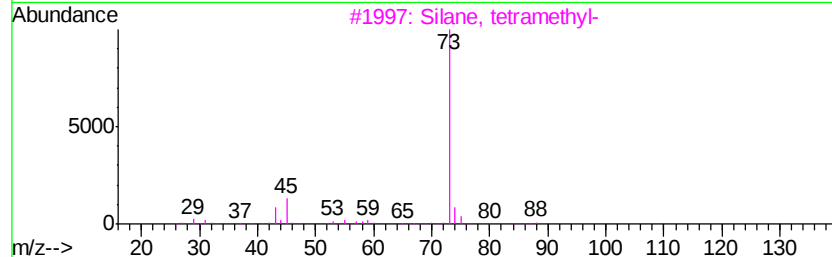
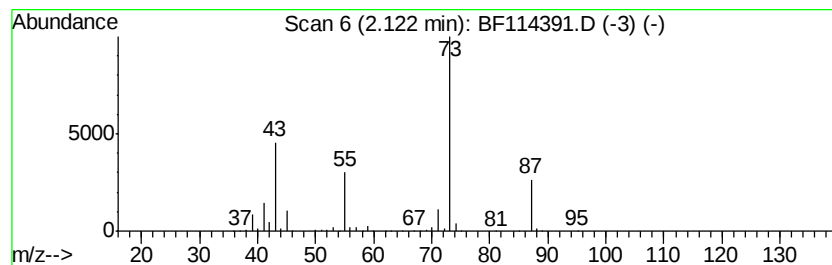
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	22.70 ng	1514040	1,4-Dichlorobenzene-d4	6.83

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		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



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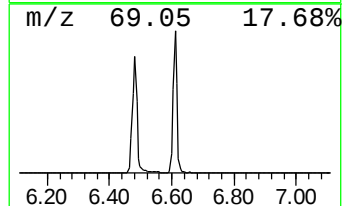
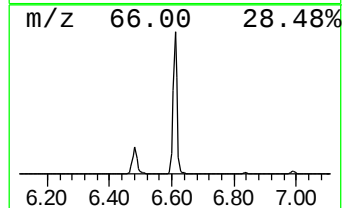
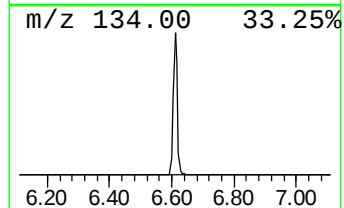
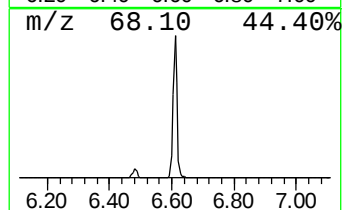
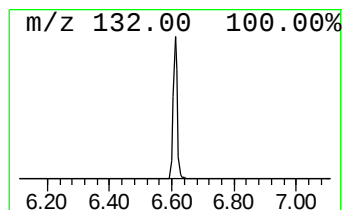
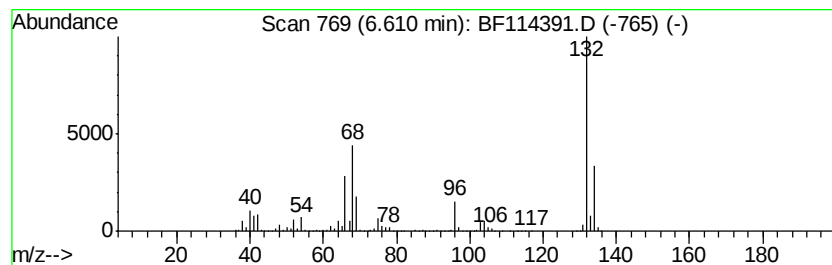
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Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	70.51 ng	4702960	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			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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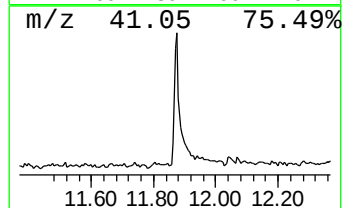
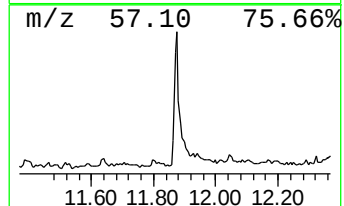
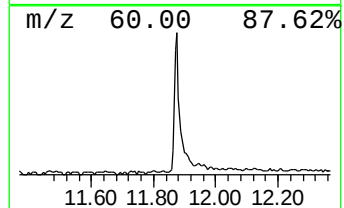
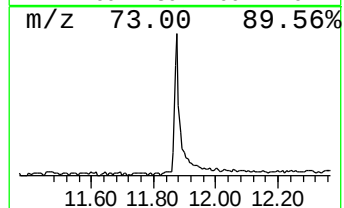
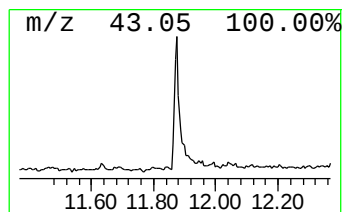
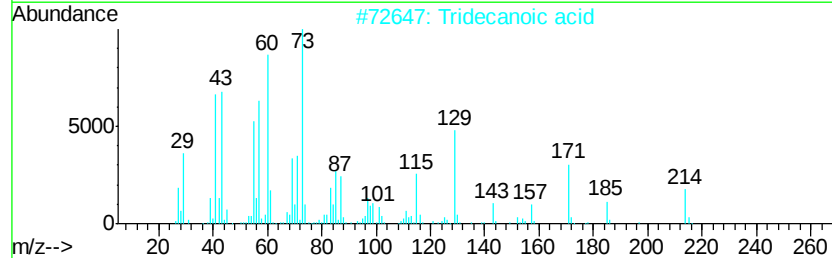
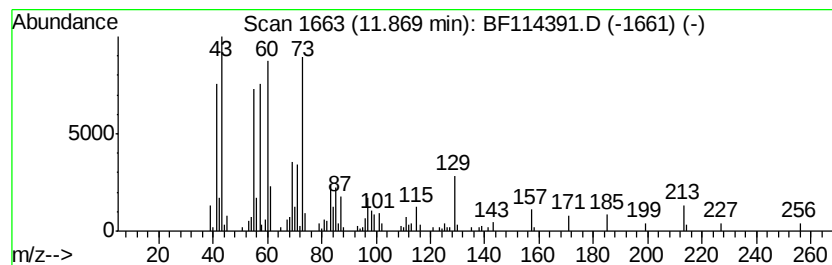
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.29 ng	340484	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	96
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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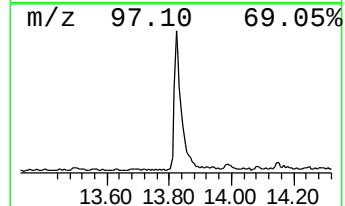
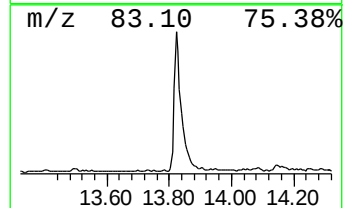
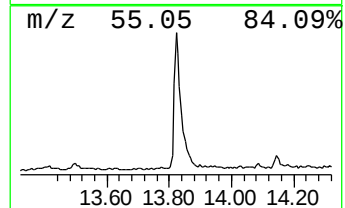
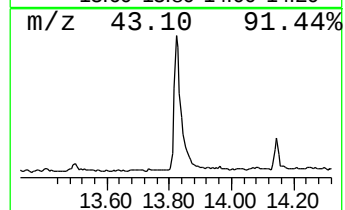
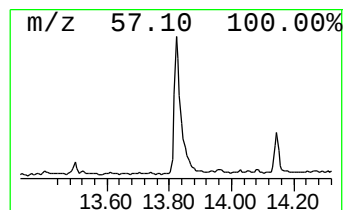
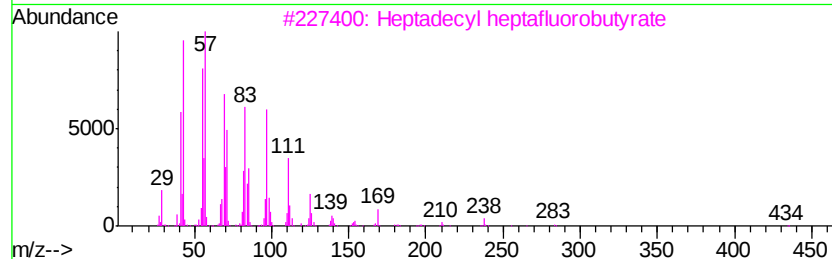
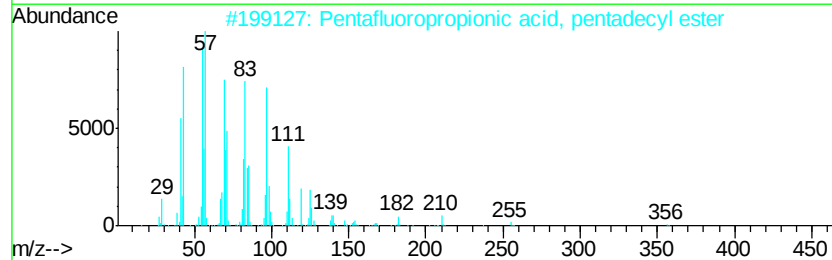
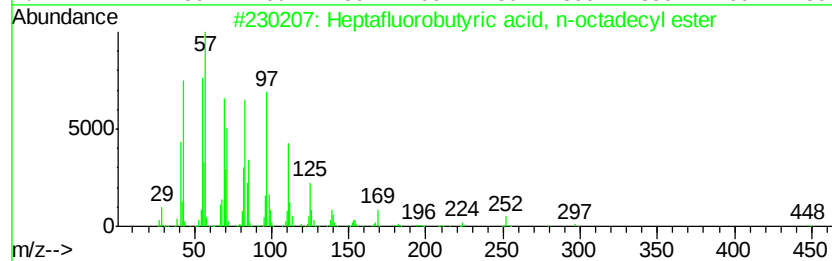
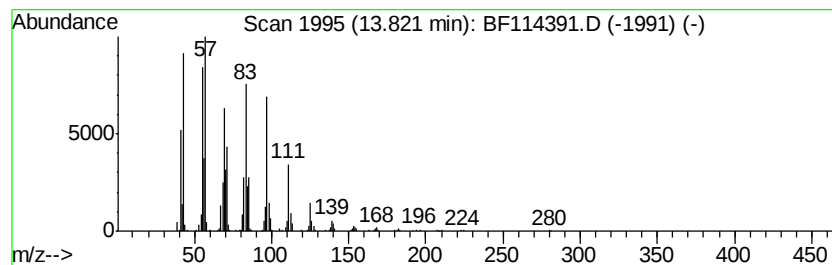
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Peak Number 5 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	12.46 ng	1080330	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		1-Docosene	308	C22H44	001599-67-3	94



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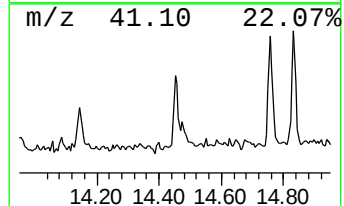
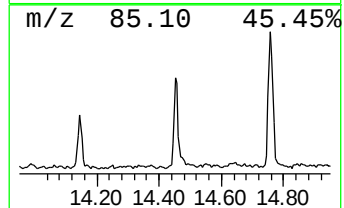
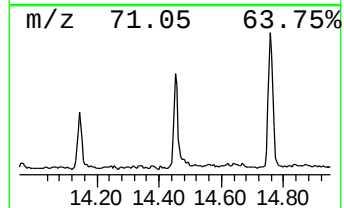
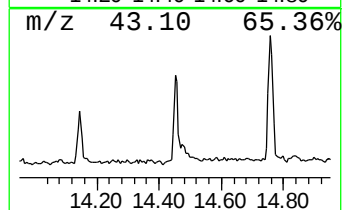
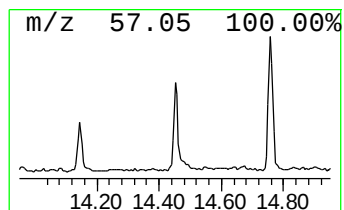
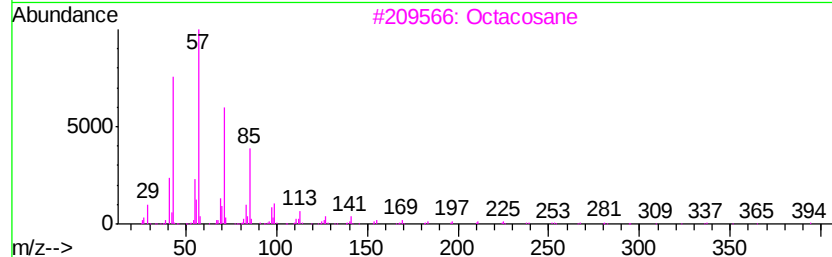
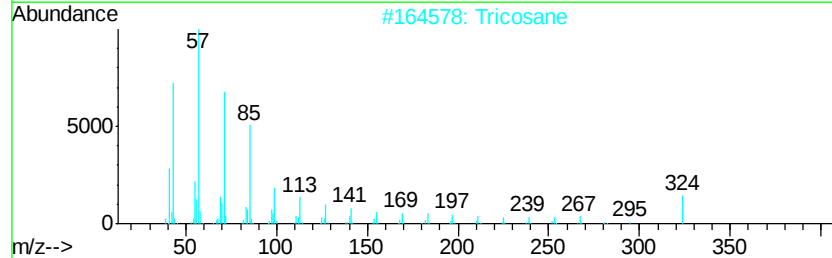
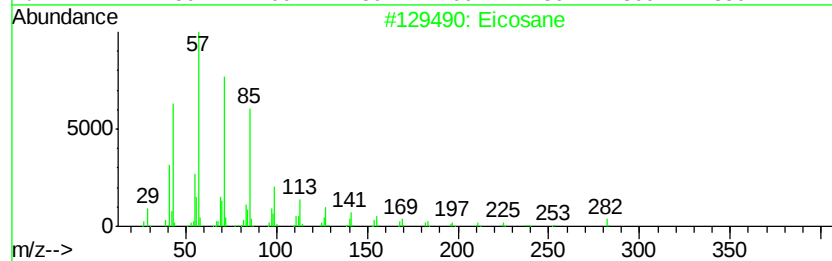
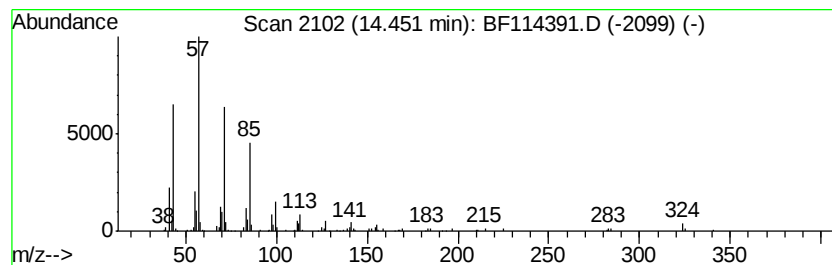
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Peak Number 6 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.47 ng	214293	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	95
2	Tricosane		324	C23H48	000638-67-5	94
3	Octacosane		394	C28H58	000630-02-4	90
4	Hexacosane		366	C26H54	000630-01-3	90
5	Tetracosane		338	C24H50	000646-31-1	87



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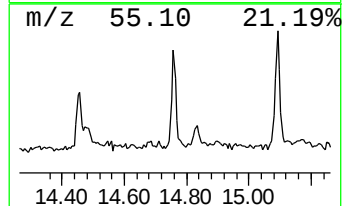
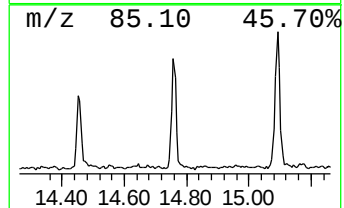
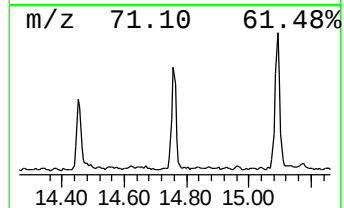
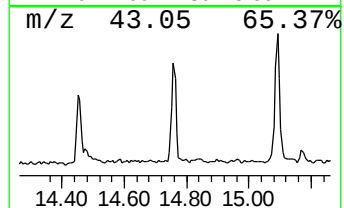
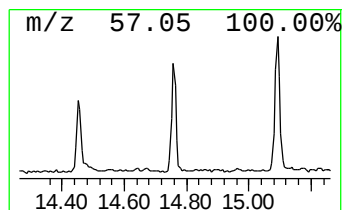
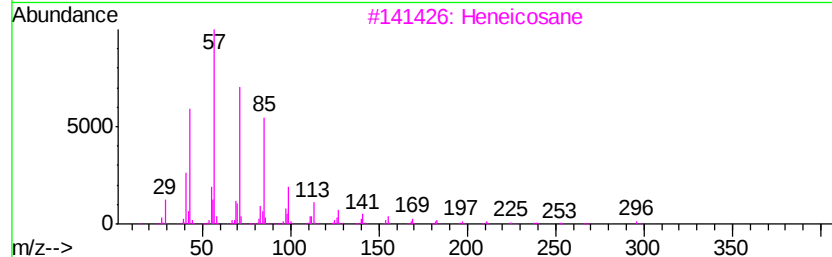
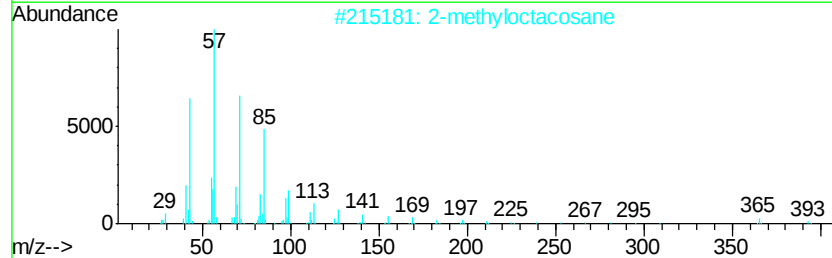
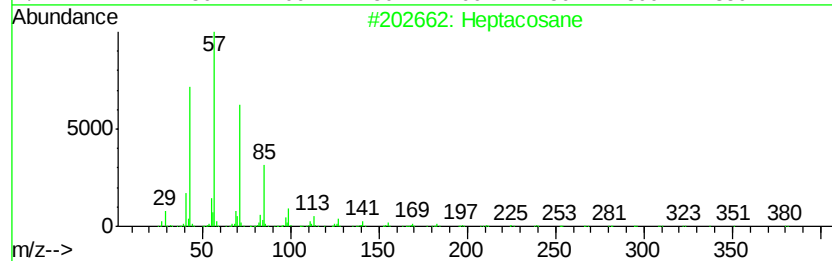
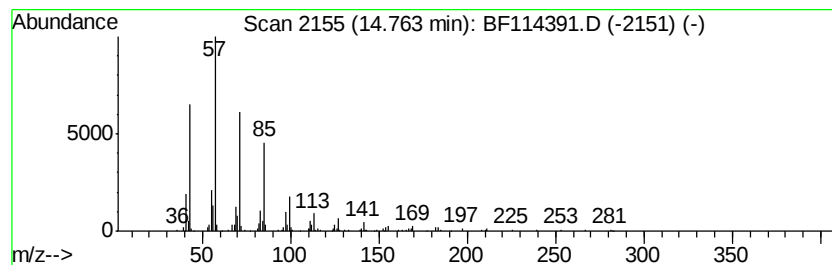
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Peak Number 7 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.50 ng	254683	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Heneicosane		296	C21H44	000629-94-7	90
4	Hexadecane		226	C16H34	000544-76-3	86
5	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114391.D
Acq On : 18 May 2019 15:18
Operator : JU/SJ
Sample : K2905-13
Misc :
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Instrument :
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ClientSampleId :
GIS-3

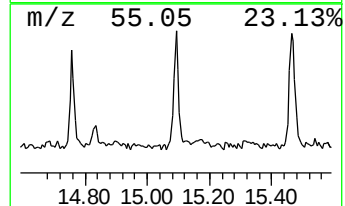
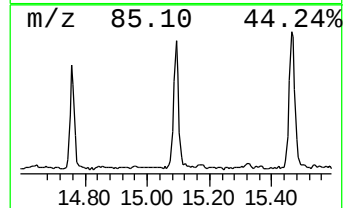
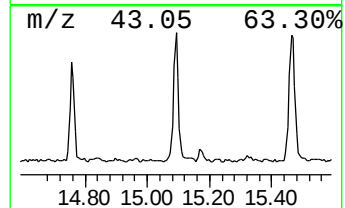
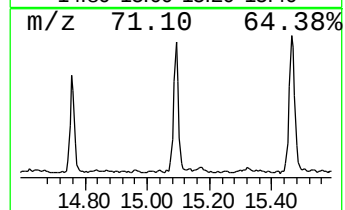
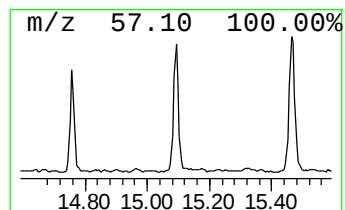
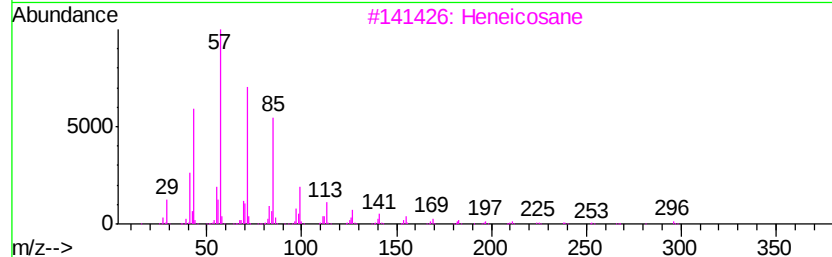
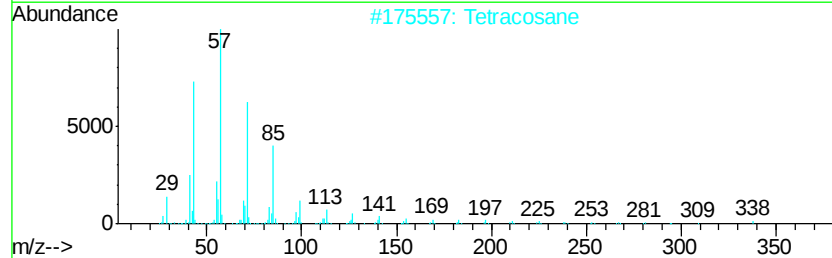
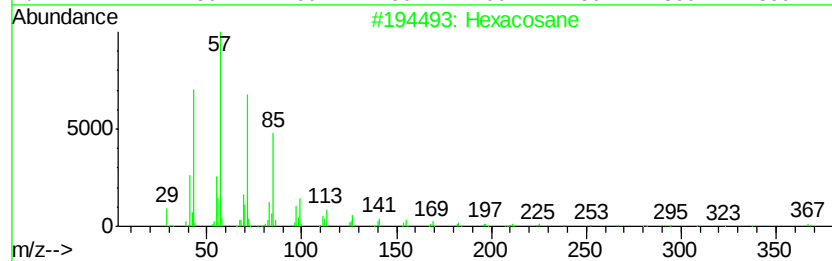
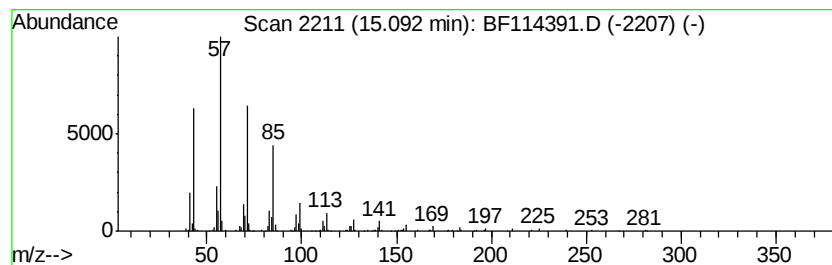
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.33 ng	339357	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	94
2	Tetracosane		338	C24H50	000646-31-1	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	Heptacosane		380	C27H56	000593-49-7	91
5	Octacosane		394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
 Data File : BF114391.D
 Acq On : 18 May 2019 15:18
 Operator : JU/SJ
 Sample : K2905-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 GIS-3

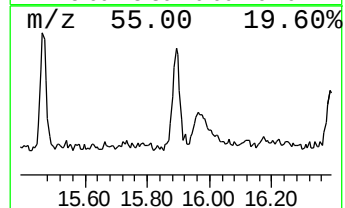
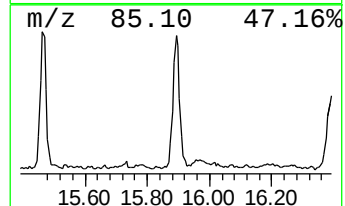
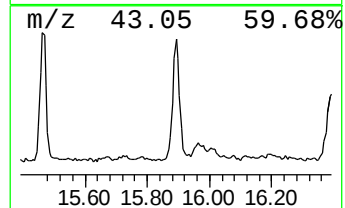
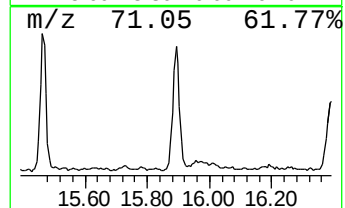
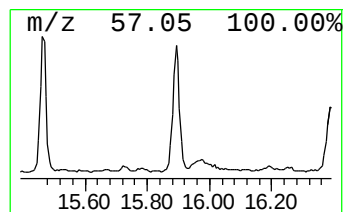
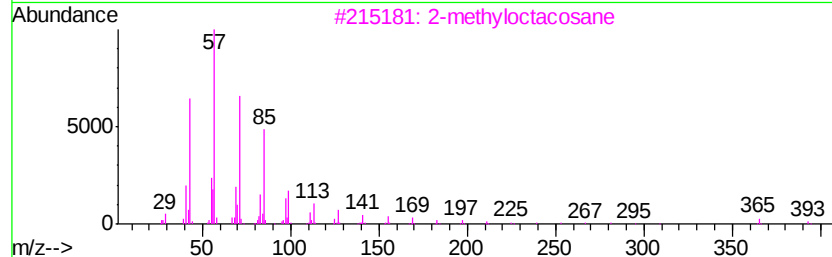
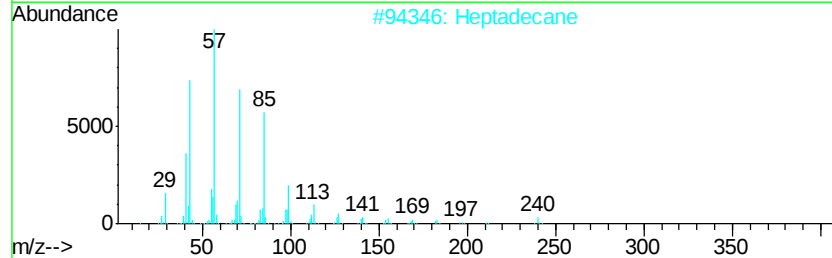
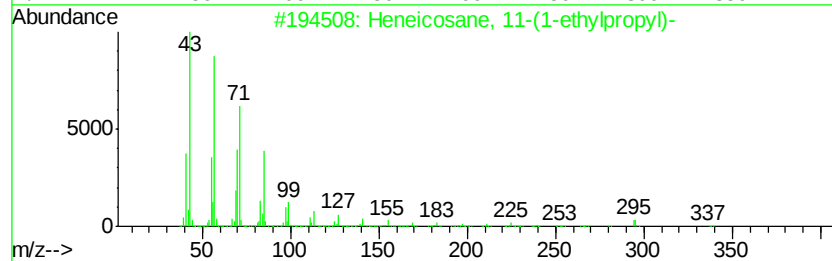
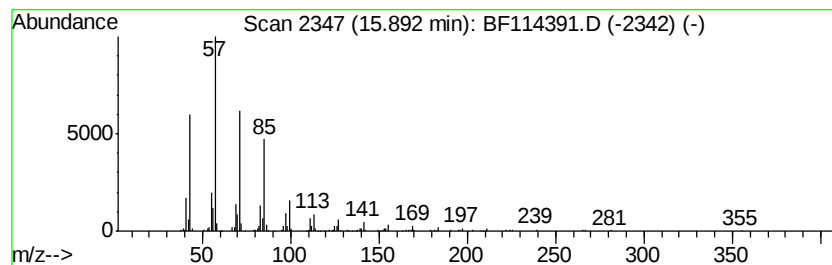
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Heneicosane, 11-(1-ethylpro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	4.60 ng	467750	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114391.D
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Operator : JU/SJ
Sample : K2905-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-3

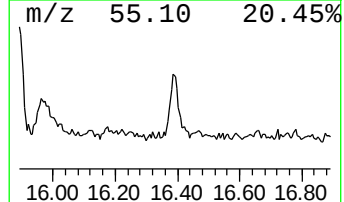
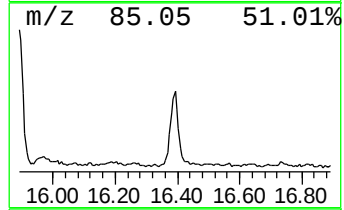
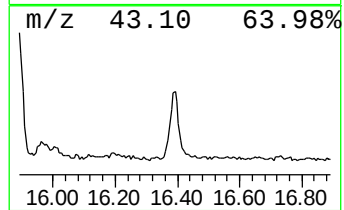
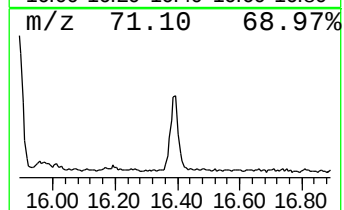
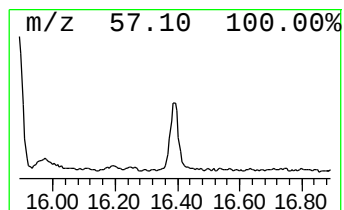
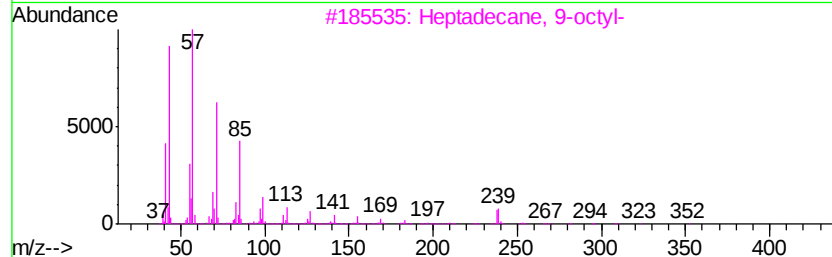
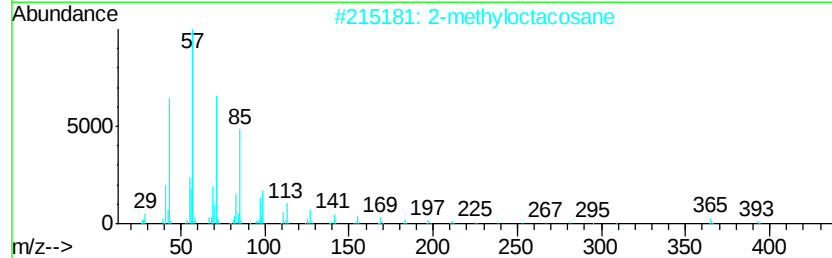
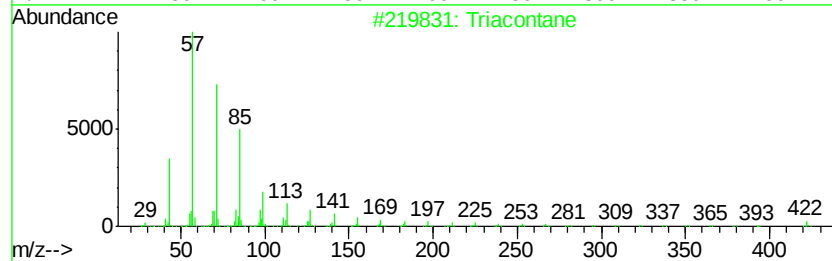
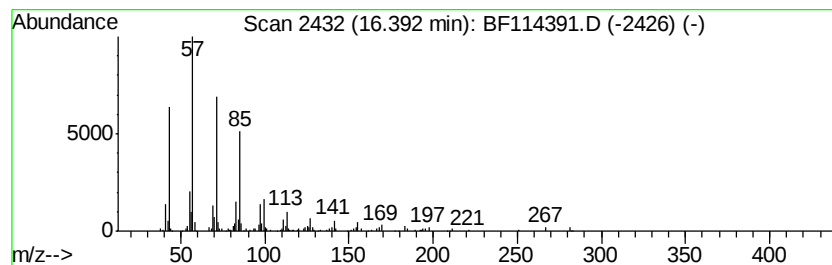
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.39	3.47 ng	353503	Perylene-d12	15.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			2-methyloctacosane	408	C29H60	1000376-72-8	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4			Heneicosane	296	C21H44	000629-94-7	87
5			Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114391.D
Acq On : 18 May 2019 15:18
Operator : JU/SJ
Sample : K2905-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GIS-3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.12	22.7	ng	1514040	1	6.83	1334070	20.0
unknown6.61	6.61	70.5	ng	4702960	1	6.83	1334070	20.0
n-Hexadecanoic acid	11.87	3.3	ng	340484	4	11.35	2070540	20.0
Heptafluorobutyri...	13.82	12.5	ng	1080330	5	13.99	1733660	20.0
Eicosane	14.45	2.5	ng	214293	5	13.99	1733660	20.0
Heptacosane	14.76	2.5	ng	254683	6	15.47	2035350	20.0
Hexacosane	15.09	3.3	ng	339357	6	15.47	2035350	20.0
Heneicosane, 11-(...	15.89	4.6	ng	467750	6	15.47	2035350	20.0
Triacontane	16.39	3.5	ng	353503	6	15.47	2035350	20.0