

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
 Data File : BF114392.D
 Acq On : 18 May 2019 15:44
 Operator : JU/SJ
 Sample : K2905-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-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	2.116	3	5	16	rVB	1003936	1128146	22.50%	2.278%
2	5.469	571	575	601	rBV	4366727	4513369	90.00%	9.112%
3	6.481	743	747	765	rBV	4592062	4784415	95.40%	9.659%
4	6.610	765	769	777	rVV	4908619	4578824	91.30%	9.244%
5	6.834	804	807	816	rBV	1527590	1307319	26.07%	2.639%
6	6.992	830	834	844	rBV	3959403	3501060	69.81%	7.068%
7	7.398	899	903	917	rBV	3053515	3002224	59.87%	6.061%
8	8.116	1021	1025	1046	rBV	1757195	1683410	33.57%	3.399%
9	9.186	1203	1207	1218	rBV	5563573	5008223	99.87%	10.111%
10	9.580	1270	1274	1284	rBV	694007	678246	13.52%	1.369%
11	9.869	1319	1323	1333	rVB	1916140	1855590	37.00%	3.746%
12	10.657	1453	1457	1472	rBV	3113575	3137162	62.56%	6.333%
13	11.351	1571	1575	1586	rBV	2174377	2037530	40.63%	4.113%
14	11.874	1660	1664	1674	rBV	327005	400873	7.99%	0.809%
15	12.657	1794	1797	1802	rBV	85355	113788	2.27%	0.230%
16	12.933	1839	1844	1847	rBV	5267916	5014871	100.00%	10.124%
17	13.157	1875	1882	1885	rBV2	54267	85981	1.71%	0.174%
18	13.827	1992	1996	2009	rBV	406919	687128	13.70%	1.387%
19	13.992	2020	2024	2032	rBV	1675560	1658270	33.07%	3.348%
20	14.145	2046	2050	2058	rVB	86409	115634	2.31%	0.233%
21	14.451	2098	2102	2113	rBV	262870	385089	7.68%	0.777%
22	14.751	2150	2153	2158	rBV	212884	222586	4.44%	0.449%
23	14.827	2163	2166	2170	rBV	62714	64256	1.28%	0.130%
24	15.086	2206	2210	2214	rBV	504113	546470	10.90%	1.103%
25	15.462	2269	2274	2283	rBV	1337171	1829674	36.48%	3.694%
26	15.656	2303	2307	2311	rBV3	70792	94383	1.88%	0.191%
27	15.886	2341	2346	2353	rBV	384313	578767	11.54%	1.168%
28	16.380	2425	2430	2436	rBV2	136121	232380	4.63%	0.469%
29	16.668	2475	2479	2487	rVB3	76111	142430	2.84%	0.288%
30	16.962	2524	2529	2536	rVB3	74825	145809	2.91%	0.294%

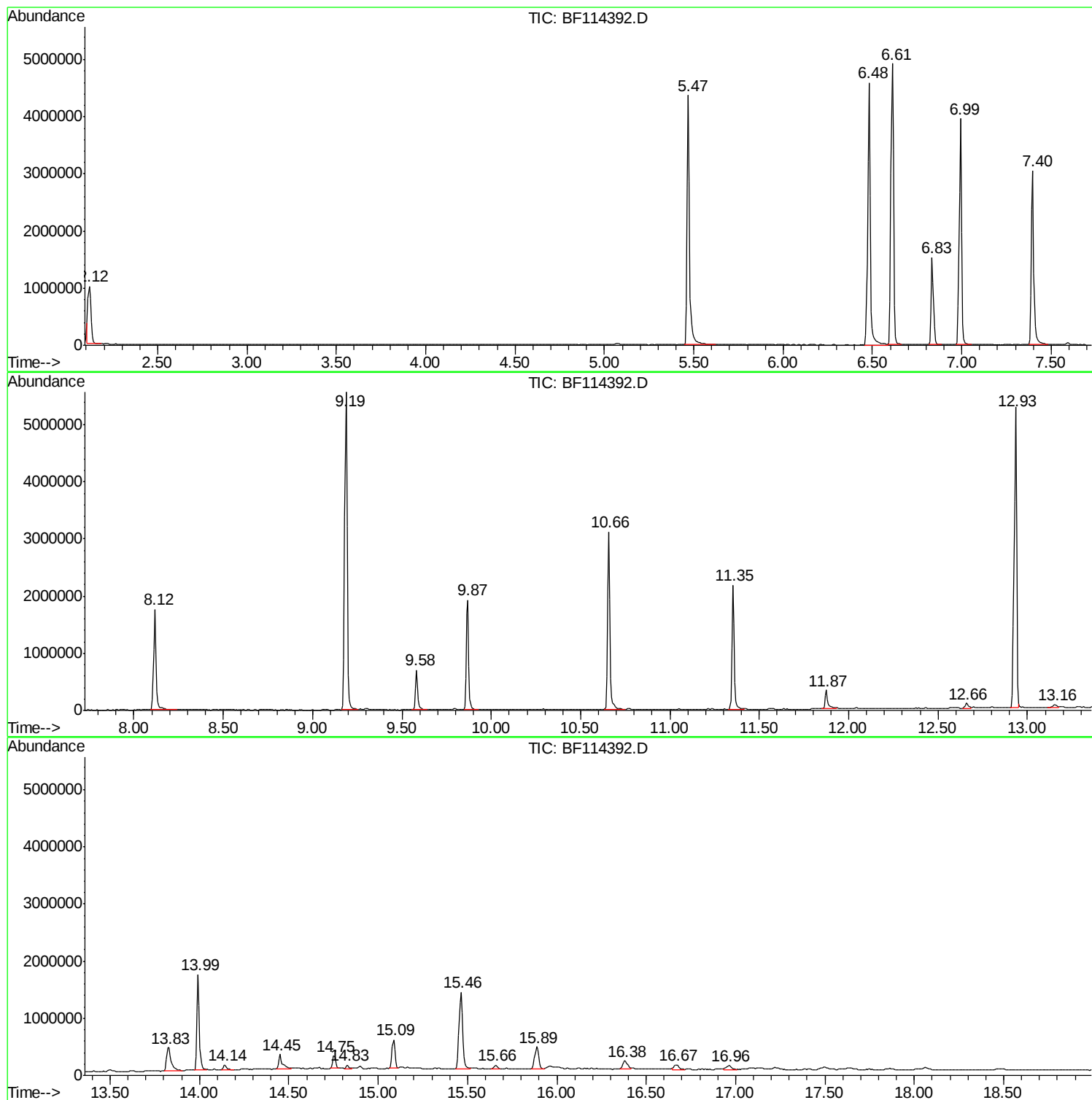
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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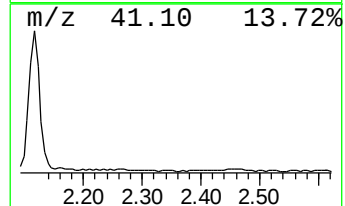
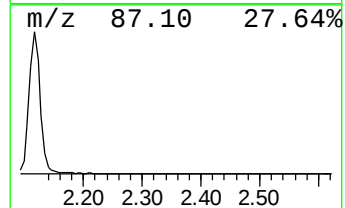
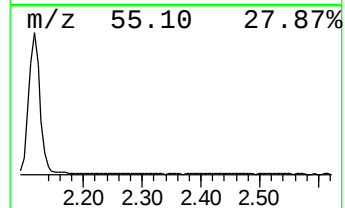
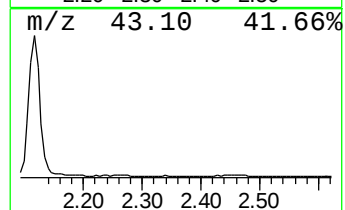
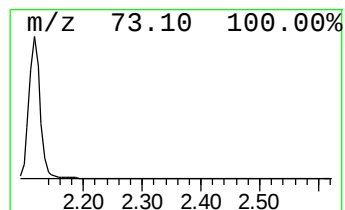
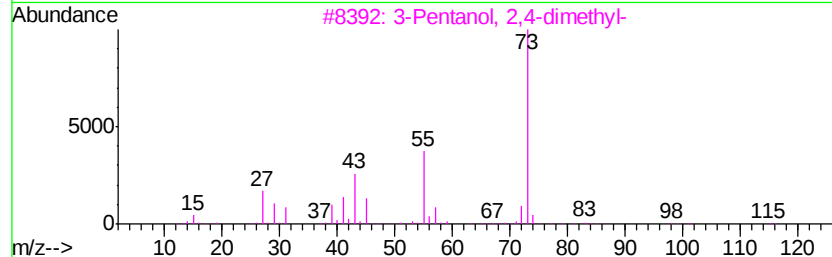
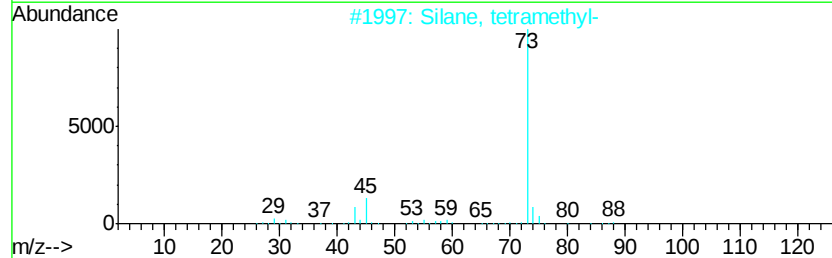
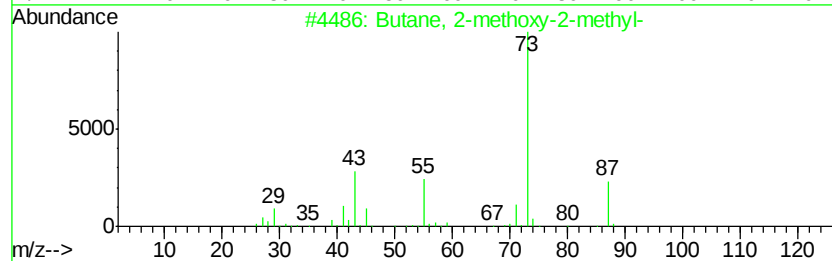
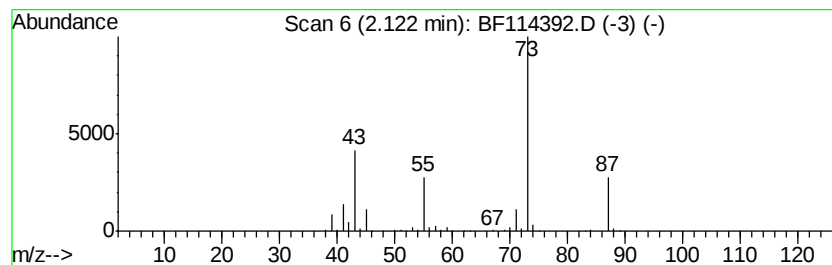
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	17.26 ng	1128150	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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10



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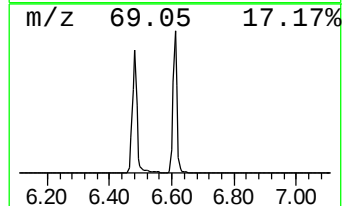
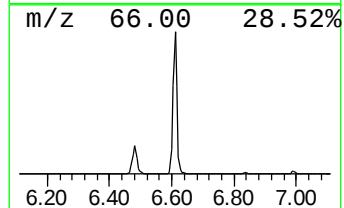
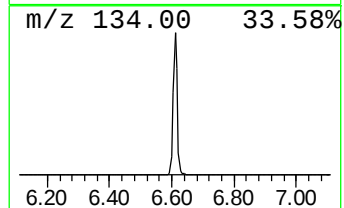
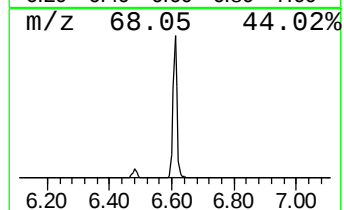
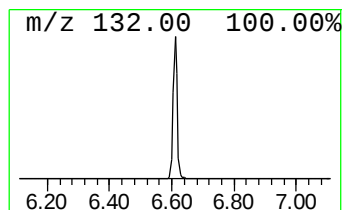
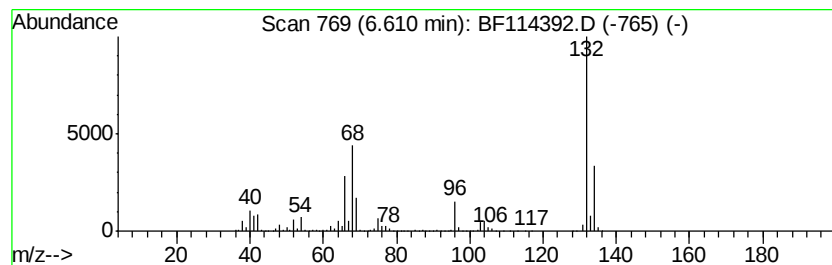
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	70.05 ng	4578820	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			Xenon	132	Xe	007440-63-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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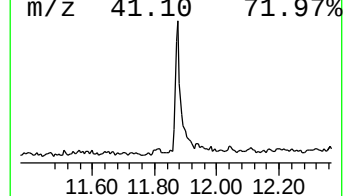
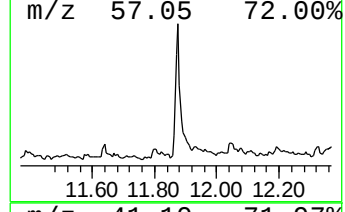
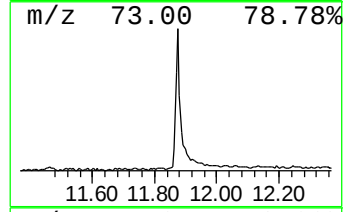
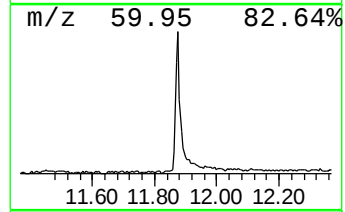
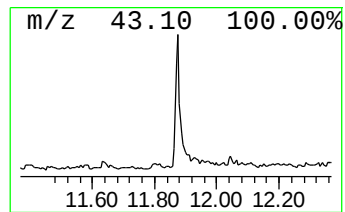
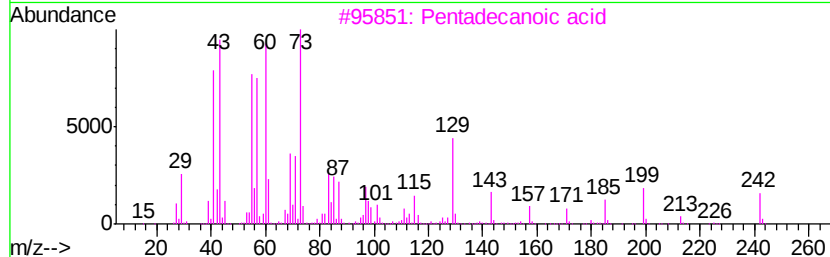
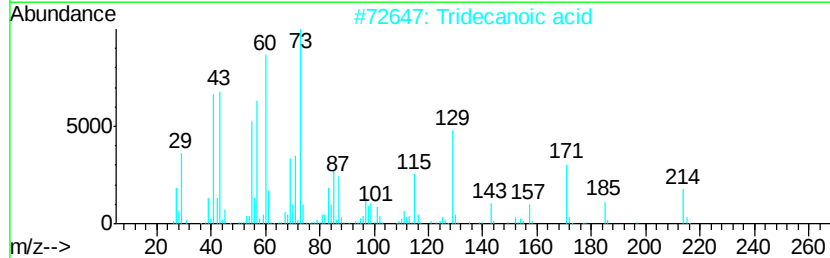
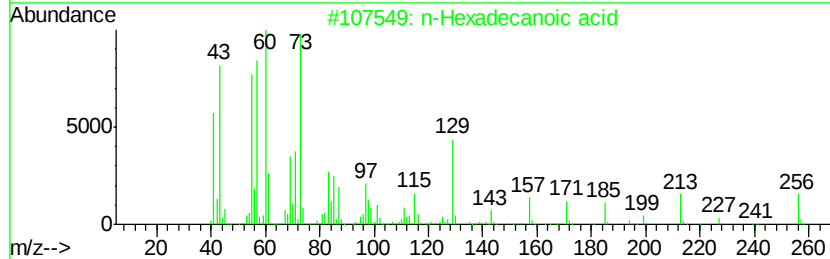
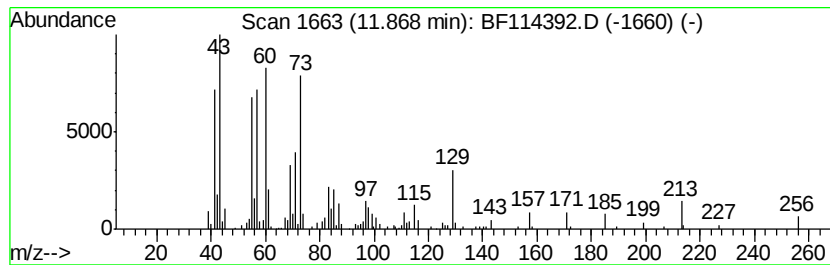
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.93 ng	400873	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	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	50



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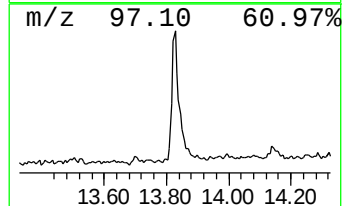
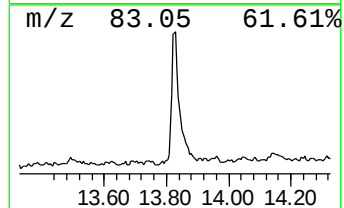
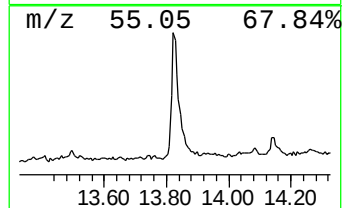
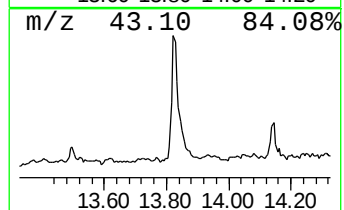
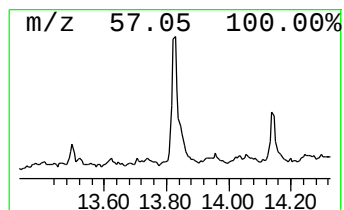
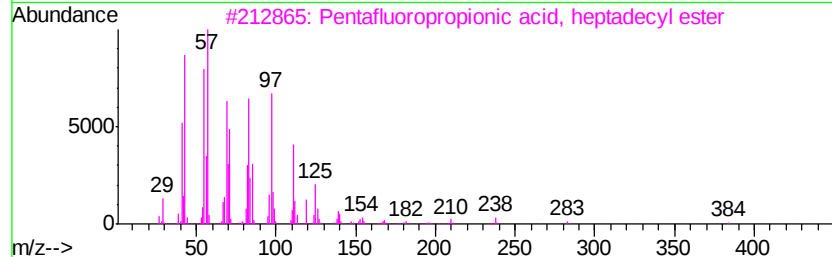
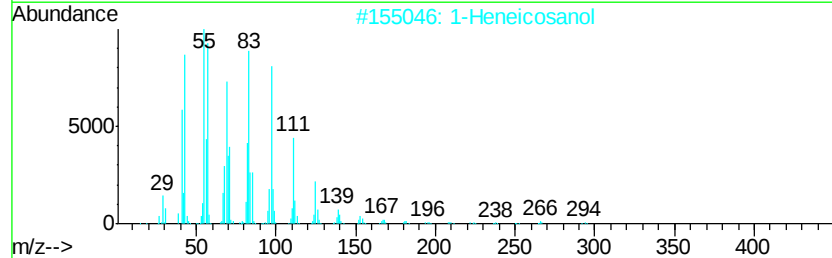
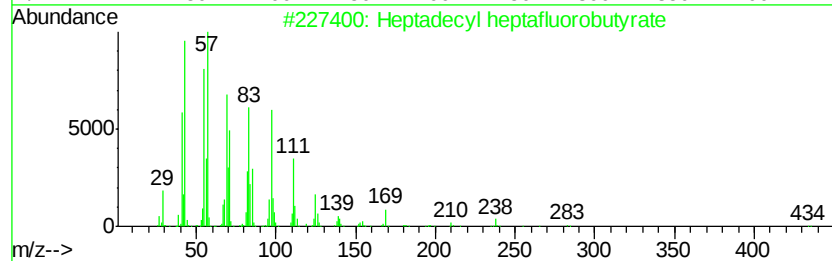
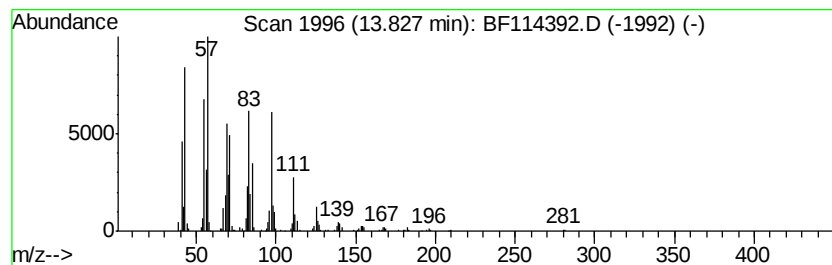
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	8.29 ng	687128	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5		Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



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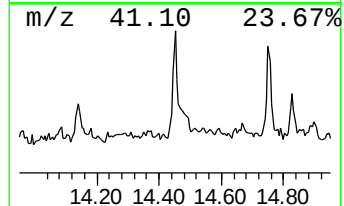
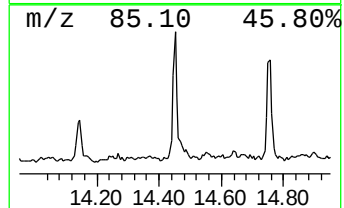
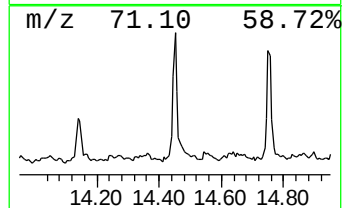
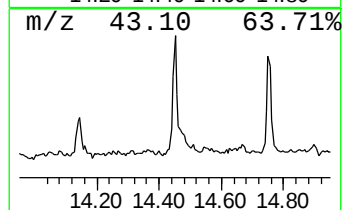
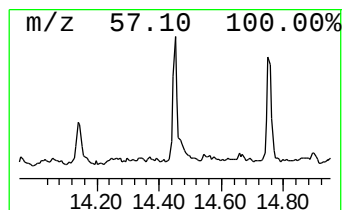
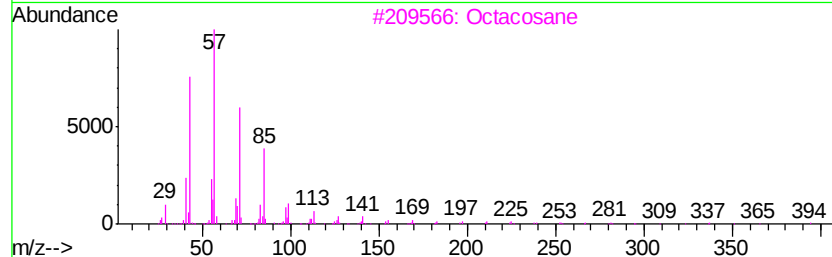
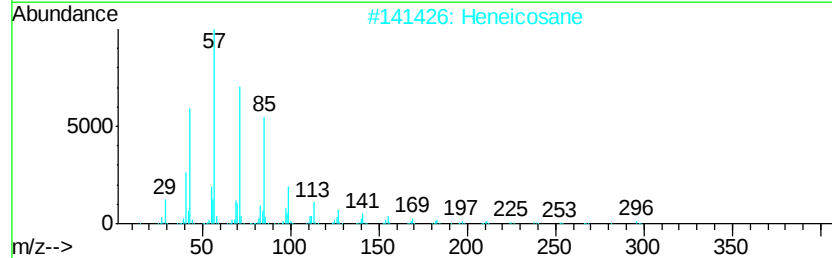
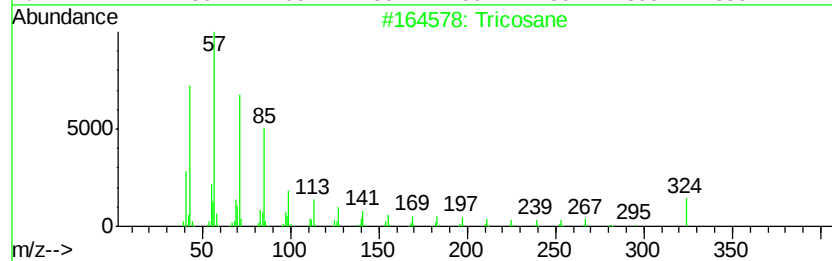
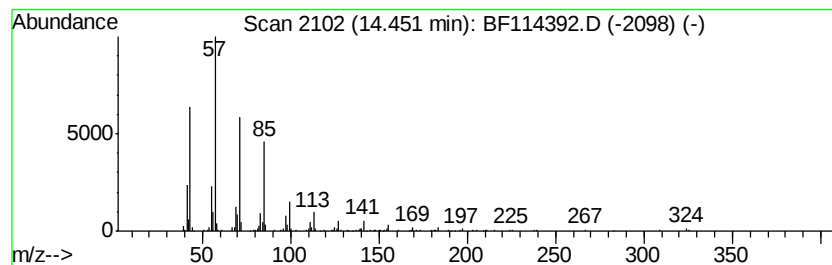
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	4.64 ng	385089	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane		324	C23H48	000638-67-5	95
2	Heneicosane		296	C21H44	000629-94-7	90
3	Octacosane		394	C28H58	000630-02-4	87
4	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	86
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	86



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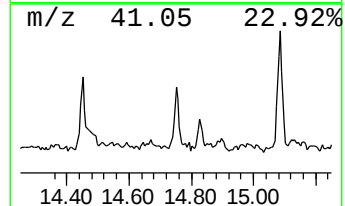
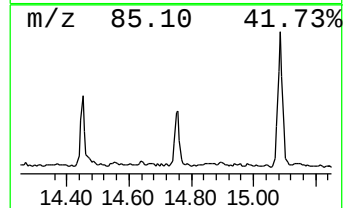
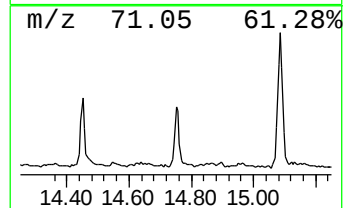
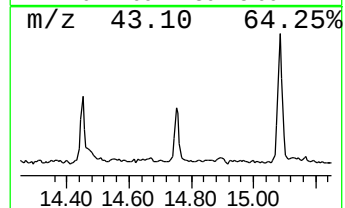
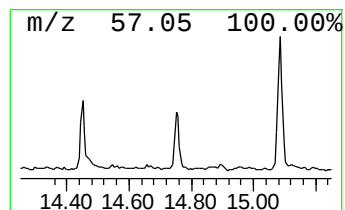
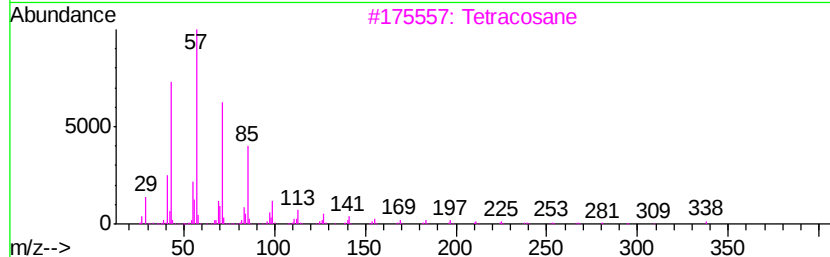
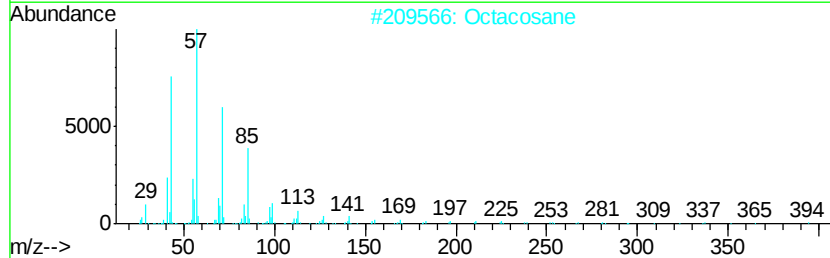
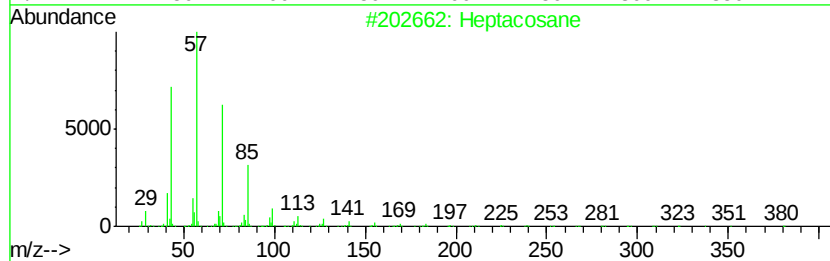
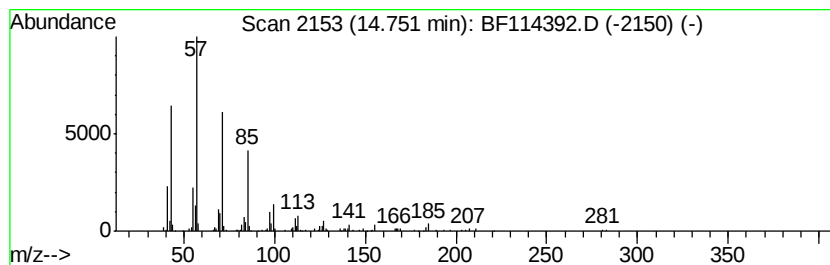
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.43 ng	222586	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Octacosane		394	C28H58	000630-02-4	90
3	Tetracosane		338	C24H50	000646-31-1	90
4	Eicosane		282	C20H42	000112-95-8	87
5	Heneicosane		296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114392.D
Acq On : 18 May 2019 15:44
Operator : JU/SJ
Sample : K2905-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-3

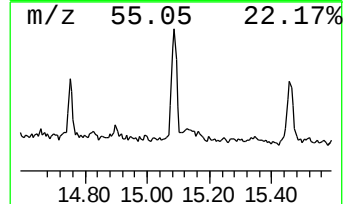
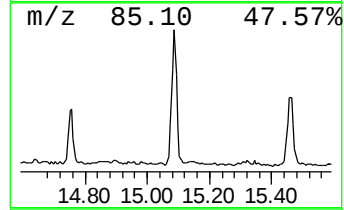
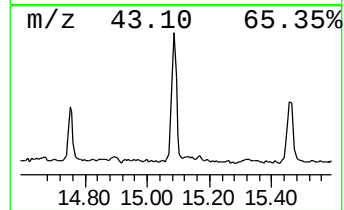
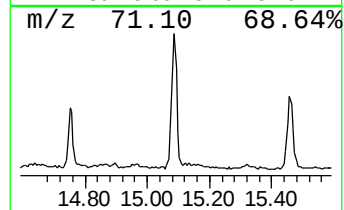
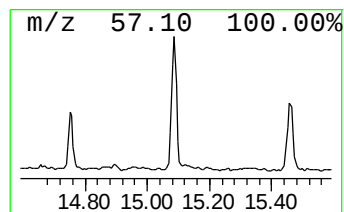
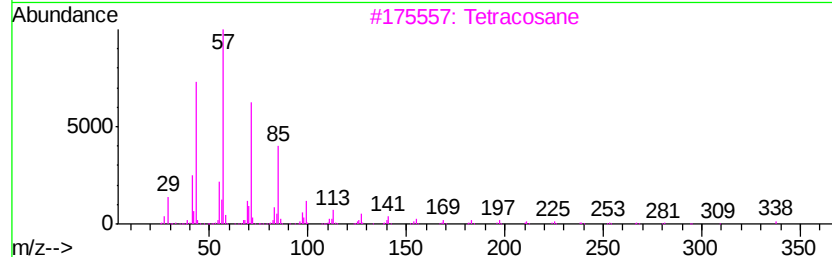
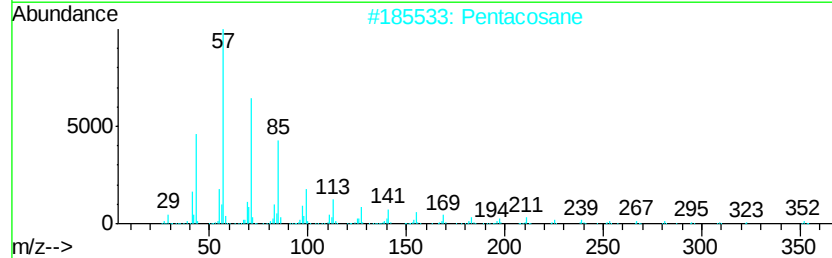
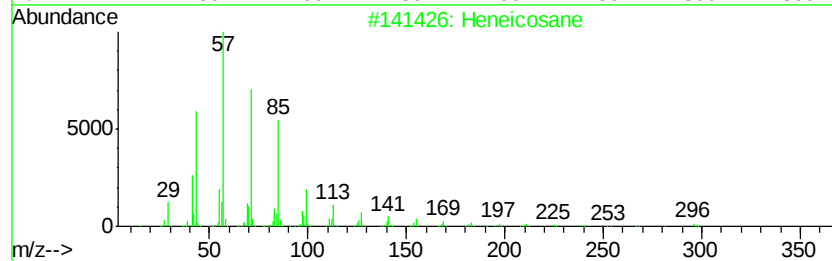
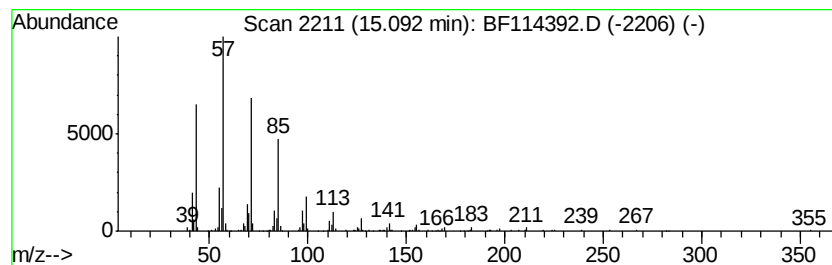
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	5.97 ng	546470	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Pentacosane		352	C25H52	000629-99-2	91
3	Tetracosane		338	C24H50	000646-31-1	90
4	2-methyloctacosane		408	C29H60	1000376-72-8	87
5	Hexadecane		226	C16H34	000544-76-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114392.D
Acq On : 18 May 2019 15:44
Operator : JU/SJ
Sample : K2905-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-3

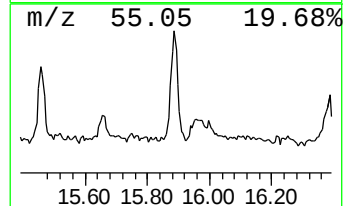
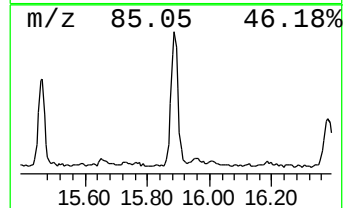
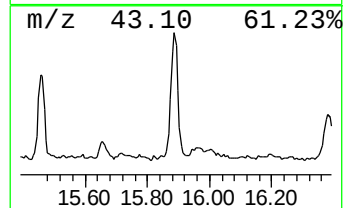
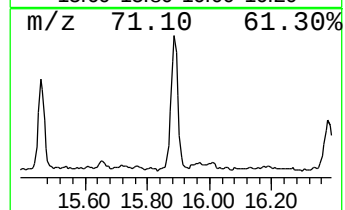
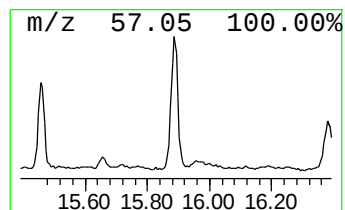
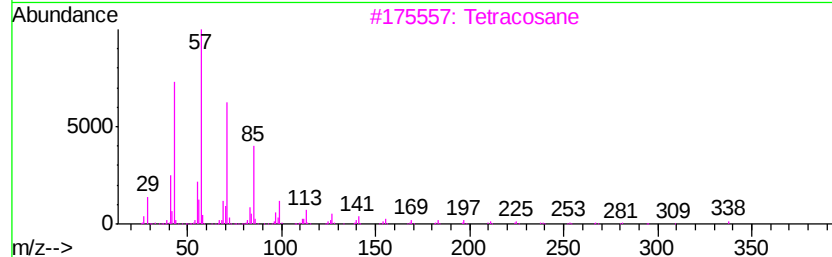
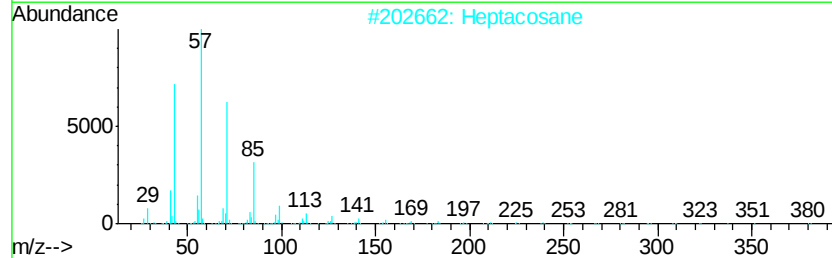
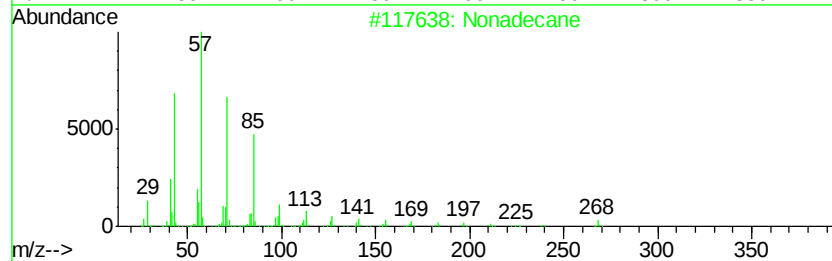
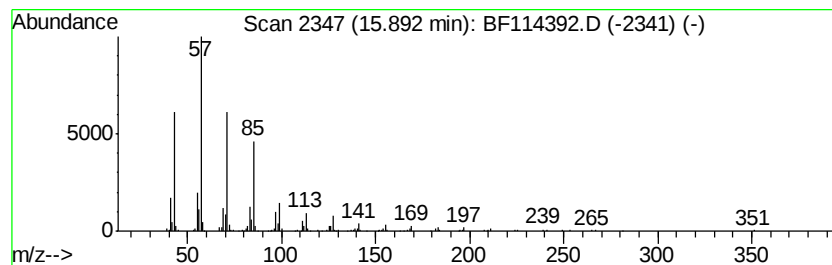
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	6.33 ng	578767	Perylene-d12	15.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	91
2	Heptacosane		380	C27H56	000593-49-7	91
3	Tetracosane		338	C24H50	000646-31-1	91
4	Hexacosane		366	C26H54	000630-01-3	90
5	Heneicosane		296	C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114392.D
Acq On : 18 May 2019 15:44
Operator : JU/SJ
Sample : K2905-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-3

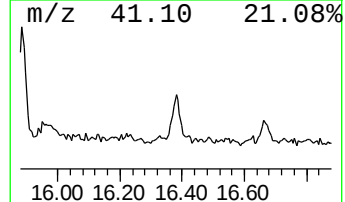
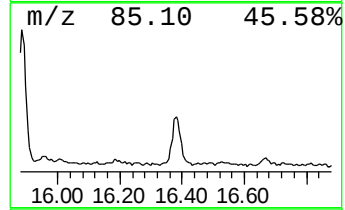
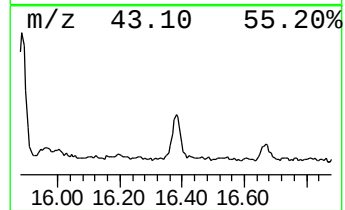
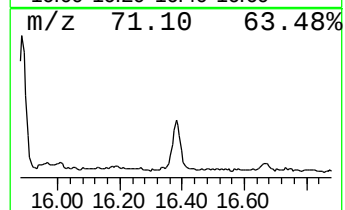
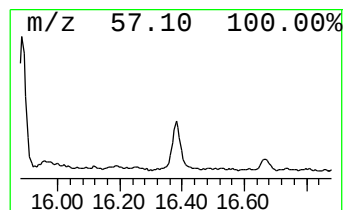
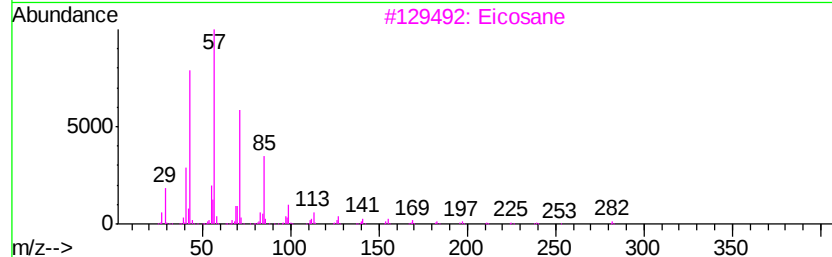
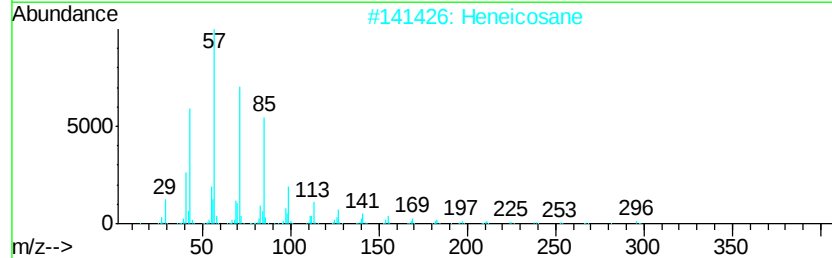
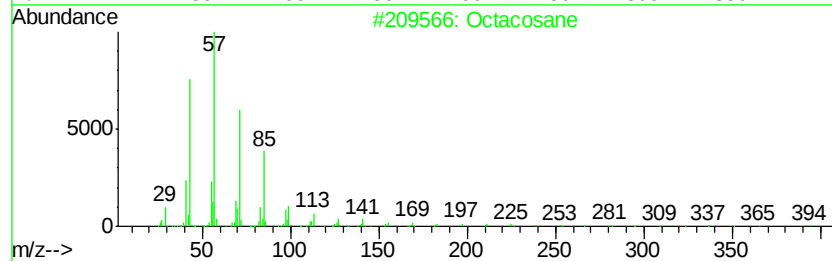
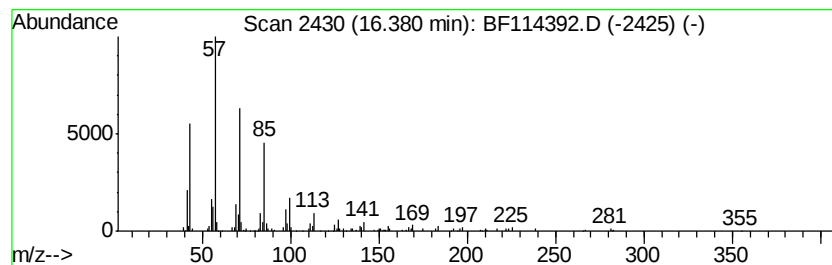
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.38	2.54 ng	232380	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Eicosane	282	C20H42	000112-95-8	87
4		Tetratetracontane	619	C44H90	007098-22-8	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114392.D
Acq On : 18 May 2019 15:44
Operator : JU/SJ
Sample : K2905-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-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
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unknown6.61	6.61	70.0	ng	4578820	1	6.83	1307320	20.0
n-Hexadecanoic acid	11.87	3.9	ng	400873	4	11.35	2037530	20.0
Heptadecyl heptaf...	13.83	8.3	ng	687128	5	13.99	1658270	20.0
Tricosane	14.45	4.6	ng	385089	5	13.99	1658270	20.0
Heptacosane	14.75	2.4	ng	222586	6	15.46	1829670	20.0
Heneicosane	15.09	6.0	ng	546470	6	15.46	1829670	20.0
Nonadecane	15.89	6.3	ng	578767	6	15.46	1829670	20.0
Octacosane	16.38	2.5	ng	232380	6	15.46	1829670	20.0