

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
 Data File : BF127599.D
 Acq On : 31 Mar 2022 12:42
 Operator : CG\JU
 Sample : N2176-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TT-156-IDWSO-20220329-1

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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127599.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.469	537	541	567	rBV	1876776	2046234	90.82%	12.852%
2	6.475	709	712	736	rBV	1958622	2109716	93.63%	13.251%
3	6.834	770	773	783	rBV	562893	464723	20.63%	2.919%
4	7.398	866	869	880	rBV	1415276	1378429	61.18%	8.658%
5	8.116	987	991	1000	rBV	646333	594577	26.39%	3.734%
6	9.186	1169	1173	1182	rBV	2347069	2224073	98.71%	13.969%
7	9.869	1286	1289	1300	rVB	789565	670021	29.74%	4.208%
8	10.663	1421	1424	1439	rBV	1338798	1397717	62.03%	8.779%
9	11.363	1540	1543	1551	rBV	791954	691632	30.70%	4.344%
10	11.733	1602	1606	1611	rVB2	24381	26628	1.18%	0.167%
11	11.880	1627	1631	1635	rBV	47217	68930	3.06%	0.433%
12	12.121	1665	1672	1690	rVB	64222	123185	5.47%	0.774%
13	12.945	1808	1812	1816	rBV	2344608	2253187	100.00%	14.152%
14	13.386	1878	1887	1897	rBV2	31703	102155	4.53%	0.642%
15	13.868	1964	1969	1982	rVB6	37531	101846	4.52%	0.640%
16	13.968	1982	1986	1990	rVB	30335	29946	1.33%	0.188%
17	14.015	1990	1994	2004	rBV	674982	644457	28.60%	4.048%
18	14.145	2012	2016	2024	rVB	52261	91132	4.04%	0.572%
19	14.233	2025	2031	2037	rVV9	20489	39413	1.75%	0.248%
20	14.751	2114	2119	2124	rBV	56362	82027	3.64%	0.515%
21	14.827	2129	2132	2136	rVB	63024	60213	2.67%	0.378%
22	15.086	2172	2176	2179	rBV	31007	38089	1.69%	0.239%
23	15.380	2222	2226	2235	rVB3	29267	54746	2.43%	0.344%
24	15.498	2242	2246	2255	rBV	457687	584474	25.94%	3.671%
25	16.562	2423	2427	2435	rVB9	20069	43756	1.94%	0.275%

Sum of corrected areas: 15921306

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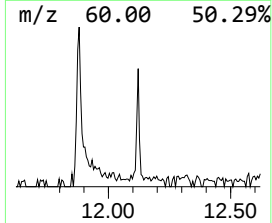
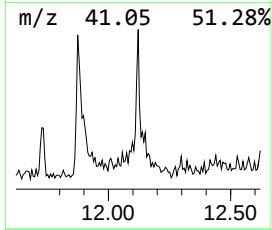
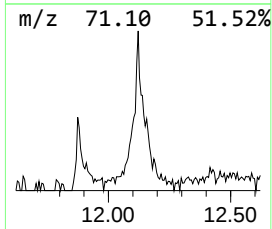
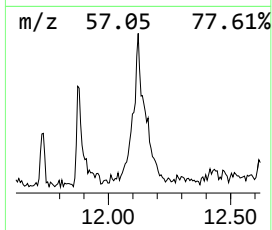
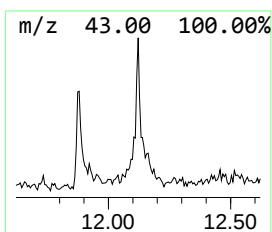
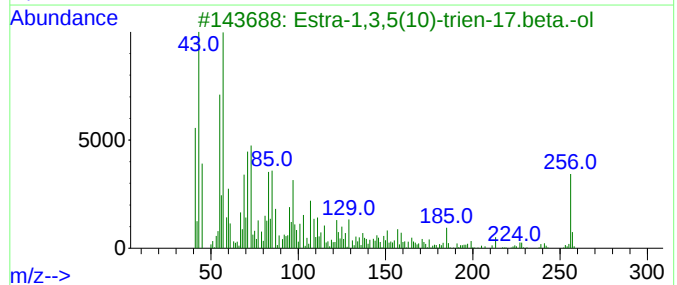
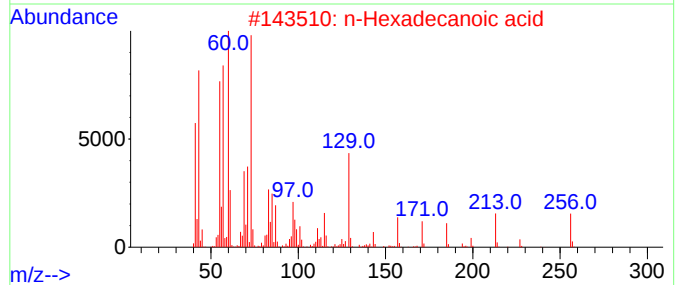
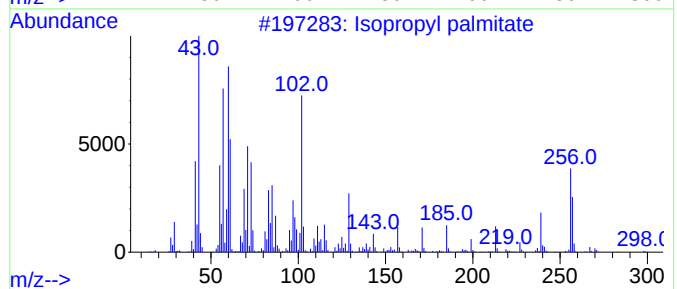
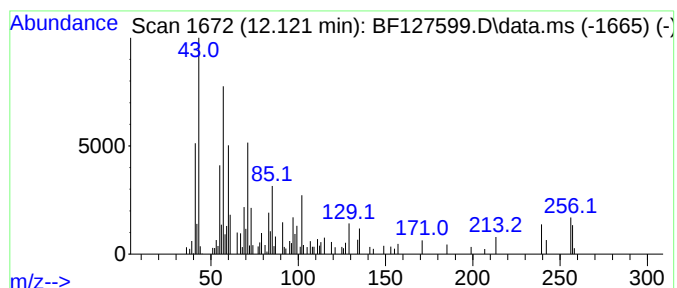
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown12.121 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.121	3.56 ng	123185	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	45
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
3			Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25
4			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	20
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	20



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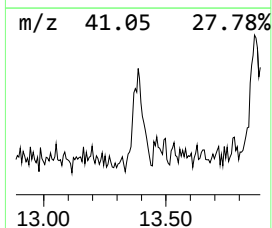
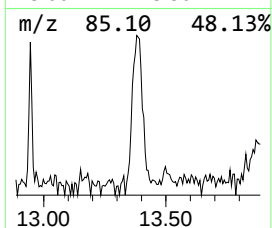
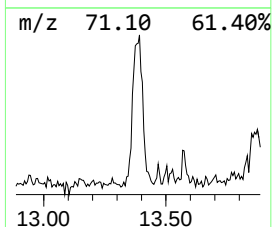
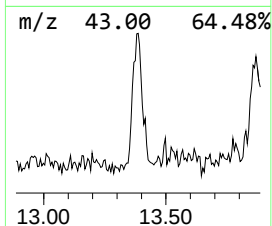
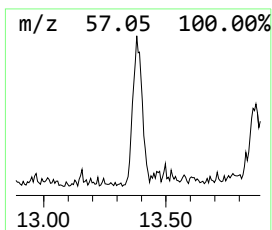
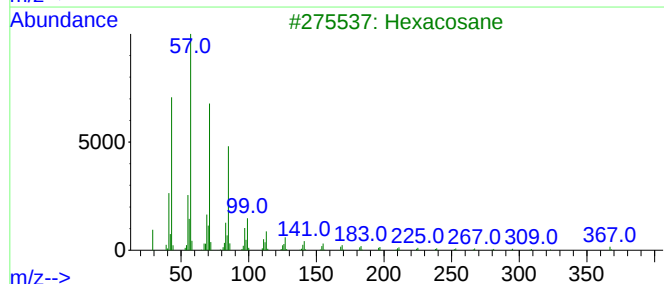
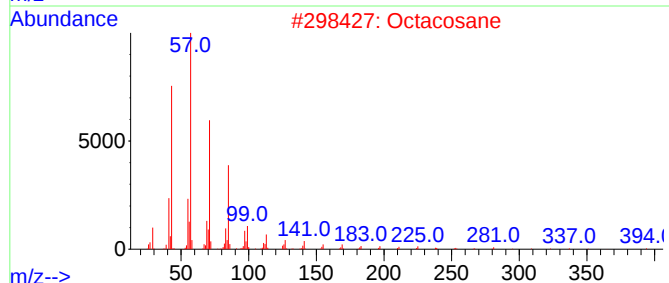
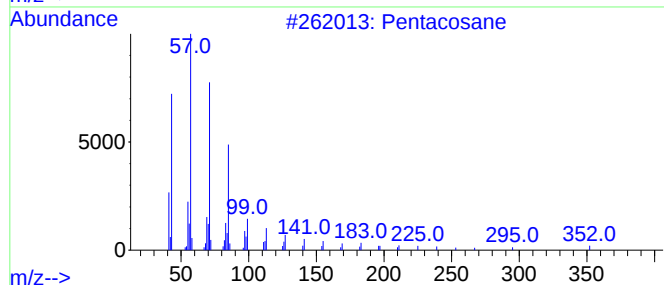
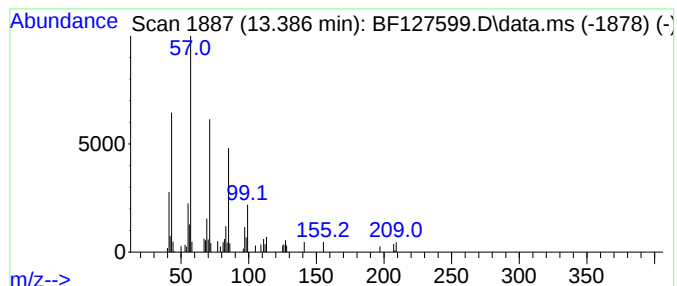
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.386	3.17 ng	102155	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	80
2			Octacosane	394	C28H58	000630-02-4	80
3			Hexacosane	366	C26H54	000630-01-3	72
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
5			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	72



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ClientSampleId :
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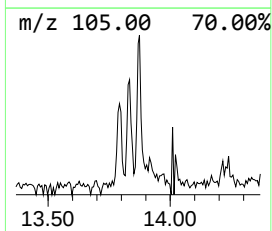
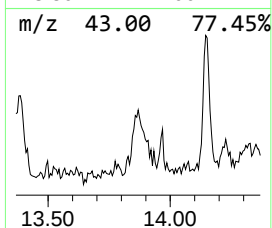
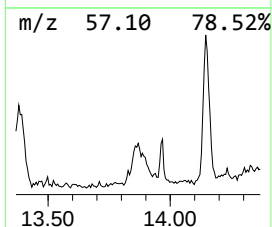
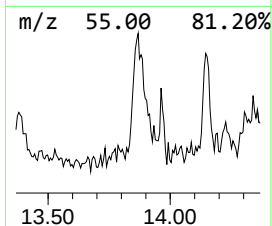
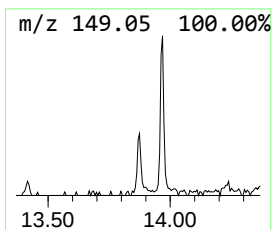
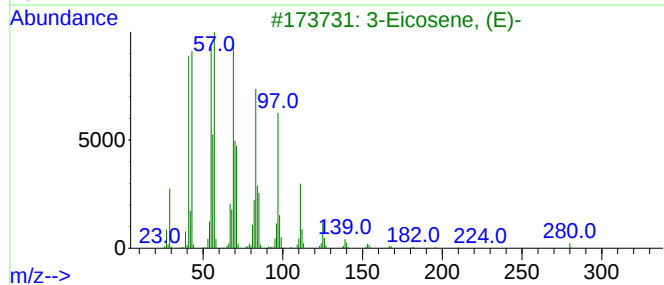
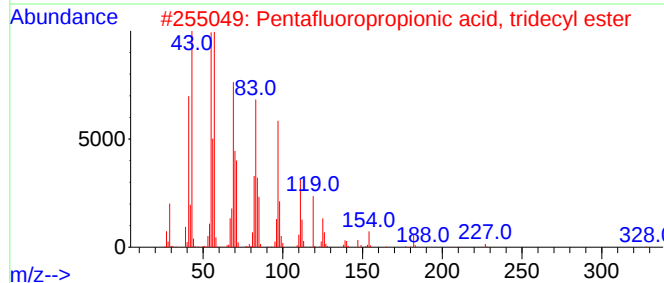
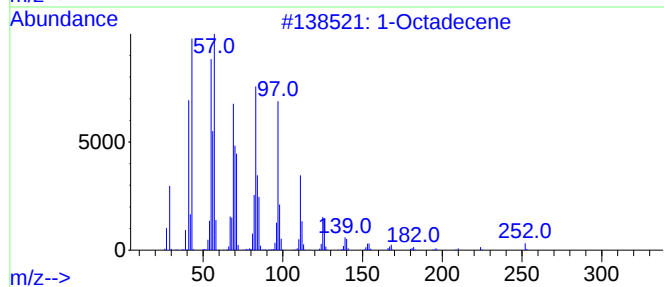
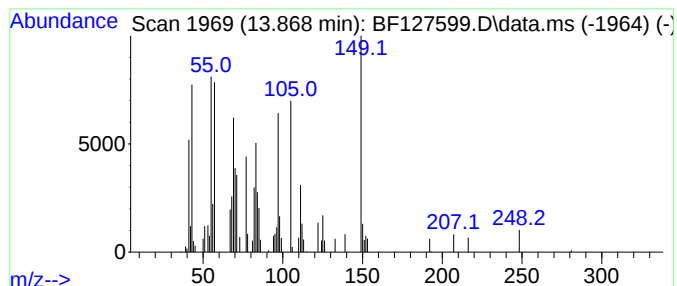
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Octadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	3.16 ng	101846	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene			252	C18H36	000112-88-9	55
2	Pentafluoropropionic acid, tridec...			346	C16H27F5O2	959261-22-4	49
3	3-Eicosene, (E)-			280	C20H40	074685-33-9	49
4	3-Octadecene, (E)-			252	C18H36	007206-19-1	49
5	1-Hexacosene			364	C26H52	018835-33-1	46



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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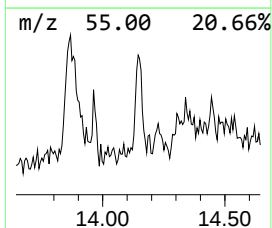
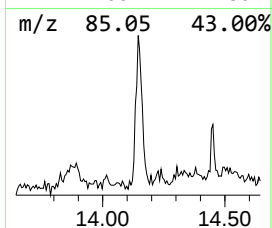
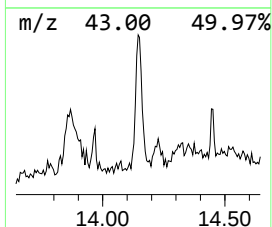
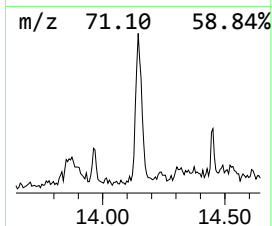
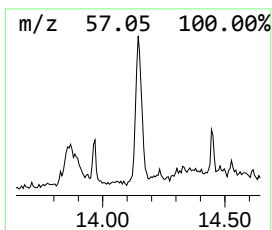
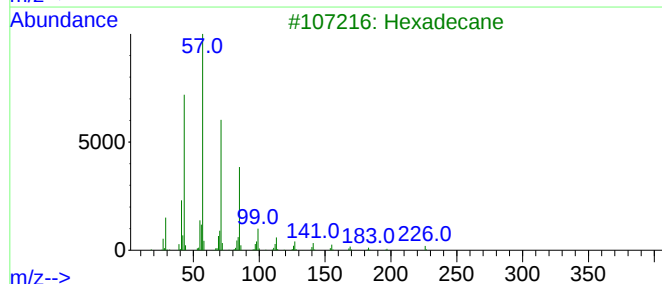
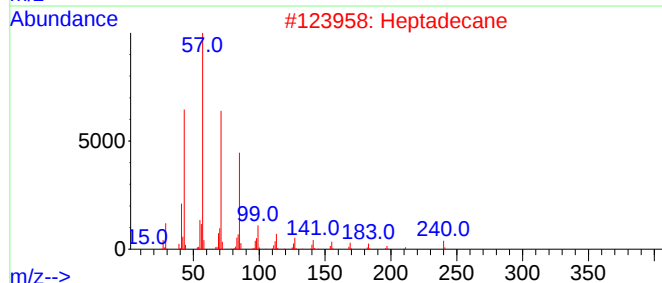
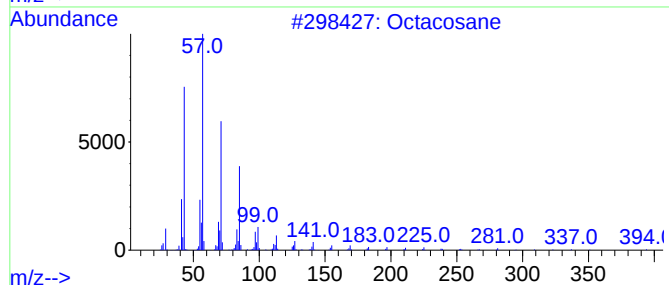
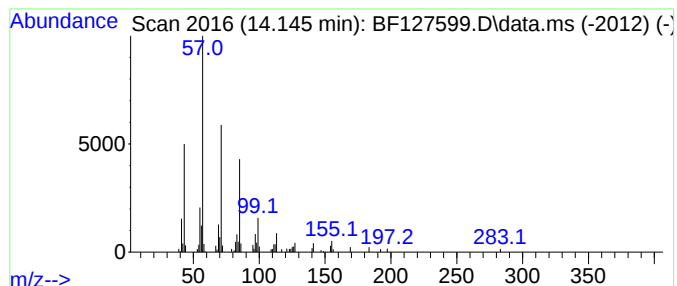
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	2.83 ng	91132	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptadecane	240	C17H36	000629-78-7	91
3			Hexadecane	226	C16H34	000544-76-3	90
4			Octadecane	254	C18H38	000593-45-3	90
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90



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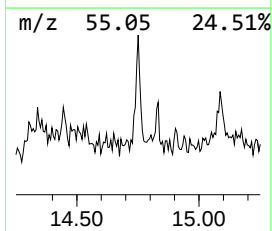
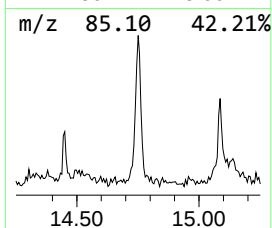
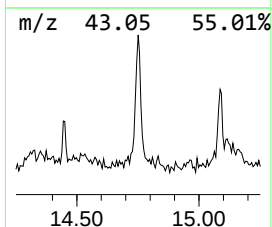
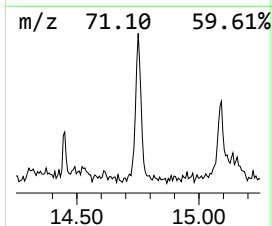
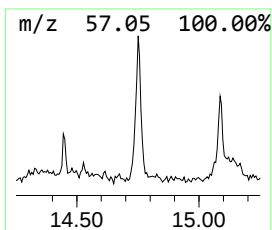
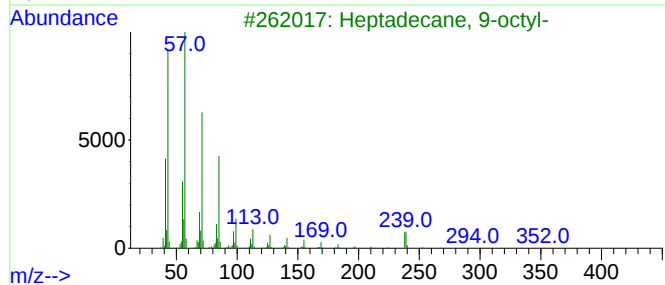
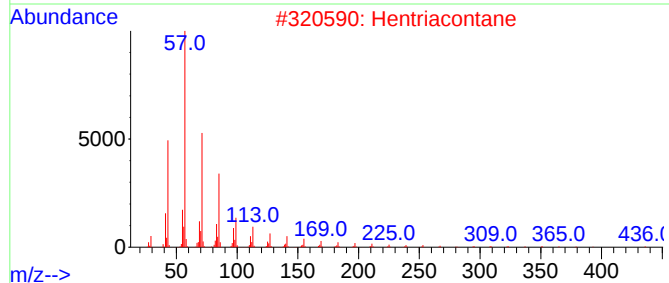
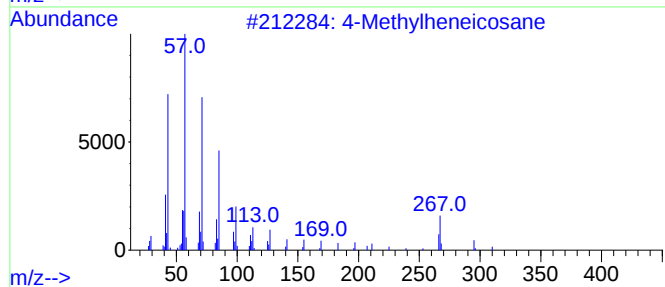
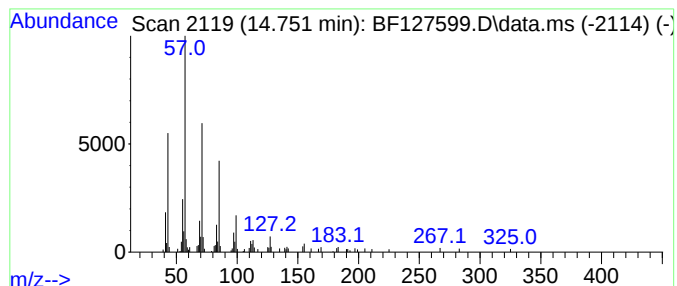
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4-Methylheneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.751	2.55 ng	82027	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methylheneicosane	310	C22H46	025117-29-7	90
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4			Heptacosane	380	C27H56	000593-49-7	86
5			Hexacosane	366	C26H54	000630-01-3	86



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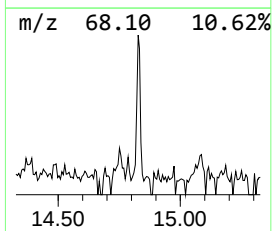
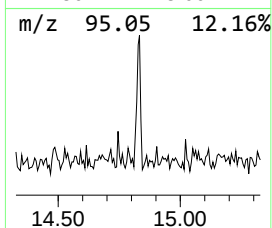
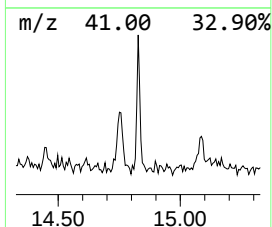
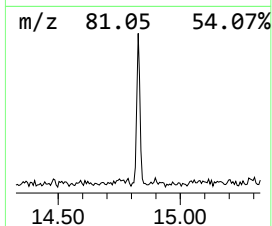
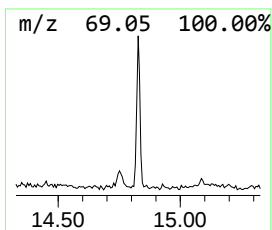
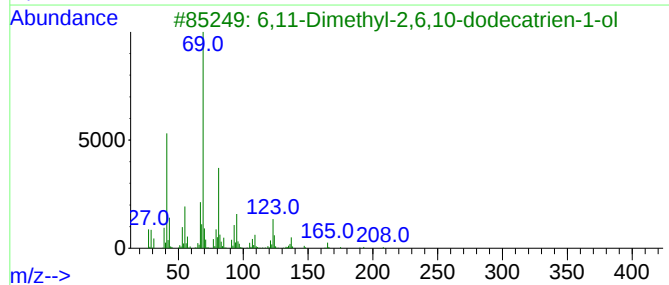
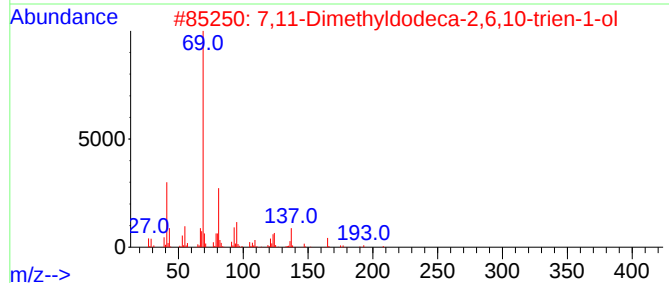
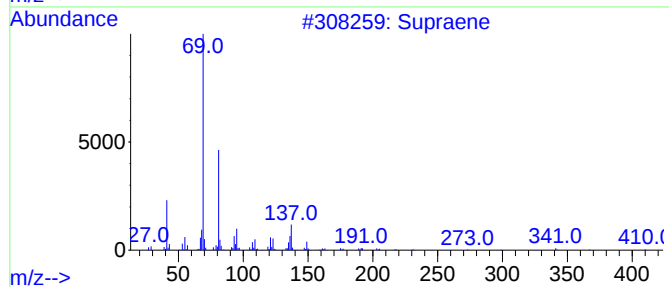
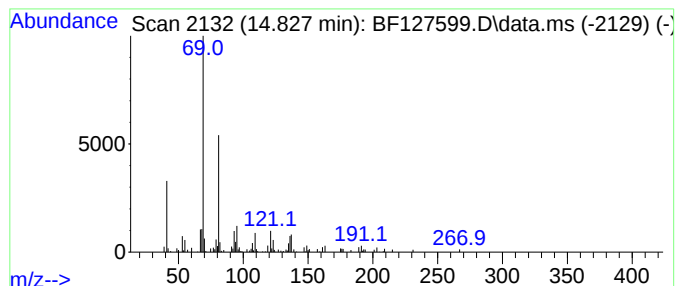
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	2.06 ng	60213	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3			6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	64
4			4,8,12-Tetradecatritienitrile, 5...	245	C17H27N	005981-31-7	64
5			4-Aza-5-thiatricyclo[5.2.1.0(3,7...	283	C14H21N03S	1000156-44-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033122\
Data File : BF127599.D
Acq On : 31 Mar 2022 12:42
Operator : CG\JU
Sample : N2176-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TT-156-IDWSO-20220329-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.121	12.121	3.6	ng	123185	4	11.363	691632	20.0
Pentacosane	13.386	3.2	ng	102155	5	14.015	644457	20.0
1-Octadecene	13.868	3.2	ng	101846	5	14.015	644457	20.0
Octacosane	14.145	2.8	ng	91132	5	14.015	644457	20.0
4-Methylheneico...	14.751	2.5	ng	82027	5	14.015	644457	20.0
Supraene	14.827	2.1	ng	60213	6	15.498	584474	20.0