

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
 Data File : BF134319.D
 Acq On : 17 Jul 2023 17:00
 Operator : CG\JU
 Sample : 03615-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-210

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	12	rVB	40811	59031	2.94%	0.388%
2	5.075	504	508	516	rVB	33518	40156	2.00%	0.264%
3	5.469	571	575	588	rBV	1879725	1726062	85.85%	11.343%
4	6.475	742	746	762	rBV	1897542	1714263	85.26%	11.265%
5	6.675	776	780	788	rBV2	16385	27907	1.39%	0.183%
6	6.834	804	807	818	rBV	570327	486838	24.21%	3.199%
7	7.398	899	903	906	rBV	1275204	1047552	52.10%	6.884%
8	8.116	1021	1025	1028	rBV	680386	591592	29.42%	3.888%
9	9.192	1204	1208	1211	rBV	2495332	2010653	100.00%	13.213%
10	9.304	1223	1227	1231	rVB	29125	26581	1.32%	0.175%
11	9.875	1320	1324	1327	rBV	757154	646829	32.17%	4.251%
12	10.081	1354	1359	1363	rBV2	22048	31539	1.57%	0.207%
13	10.586	1440	1445	1449	rVB2	29178	33170	1.65%	0.218%
14	10.669	1455	1459	1472	rBV	1324819	1256229	62.48%	8.255%
15	11.369	1574	1578	1580	rBV	588228	509049	25.32%	3.345%
16	11.392	1580	1582	1586	rVB	86678	75850	3.77%	0.498%
17	11.604	1614	1618	1624	rBV6	14675	34641	1.72%	0.228%
18	11.869	1661	1663	1665	rBV	26476	26825	1.33%	0.176%
19	11.898	1665	1668	1672	rVV2	318636	297743	14.81%	1.957%
20	11.980	1680	1682	1685	rBV2	34526	34023	1.69%	0.224%
21	12.316	1734	1739	1741	rBV4	24605	36922	1.84%	0.243%
22	12.422	1754	1757	1760	rBV	52187	51760	2.57%	0.340%
23	12.457	1760	1763	1766	rVV3	34571	42322	2.10%	0.278%
24	12.516	1770	1773	1777	rBV	38516	43037	2.14%	0.283%
25	12.586	1782	1785	1789	rBV	310403	299817	14.91%	1.970%
26	12.686	1799	1802	1807	rBV2	113721	128192	6.38%	0.842%
27	12.822	1819	1825	1832	rBV	273087	324744	16.15%	2.134%
28	12.875	1832	1834	1838	rVB2	27109	29140	1.45%	0.191%
29	12.963	1845	1849	1856	rVB	2063022	1836150	91.32%	12.066%
30	13.039	1858	1862	1866	rBV4	26474	47786	2.38%	0.314%
31	13.133	1874	1878	1879	rBV3	29207	38855	1.93%	0.255%
32	13.151	1879	1881	1885	rVB	50120	47214	2.35%	0.310%
33	13.216	1890	1892	1895	rVV	30507	31321	1.56%	0.206%
34	13.257	1896	1899	1901	rVB2	28697	27659	1.38%	0.182%
35	13.345	1912	1914	1917	rBV	21692	23992	1.19%	0.158%
36	13.669	1966	1969	1972	rVB	36430	36856	1.83%	0.242%

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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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.874	2002	2004	2005	rBV2	32661	27578	1.37%	0.181%
38	14.027	2023	2030	2033	rBV2	572288	704930	35.06%	4.632%
39	14.051	2033	2034	2038	rVB	144056	114019	5.67%	0.749%
40	14.886	2173	2176	2180	rVB	81142	84460	4.20%	0.555%
41	15.086	2207	2210	2213	rBV	97380	127875	6.36%	0.840%
42	15.527	2281	2285	2295	rVB	248673	393251	19.56%	2.584%
43	16.010	2365	2367	2371	rBV	34729	42736	2.13%	0.281%

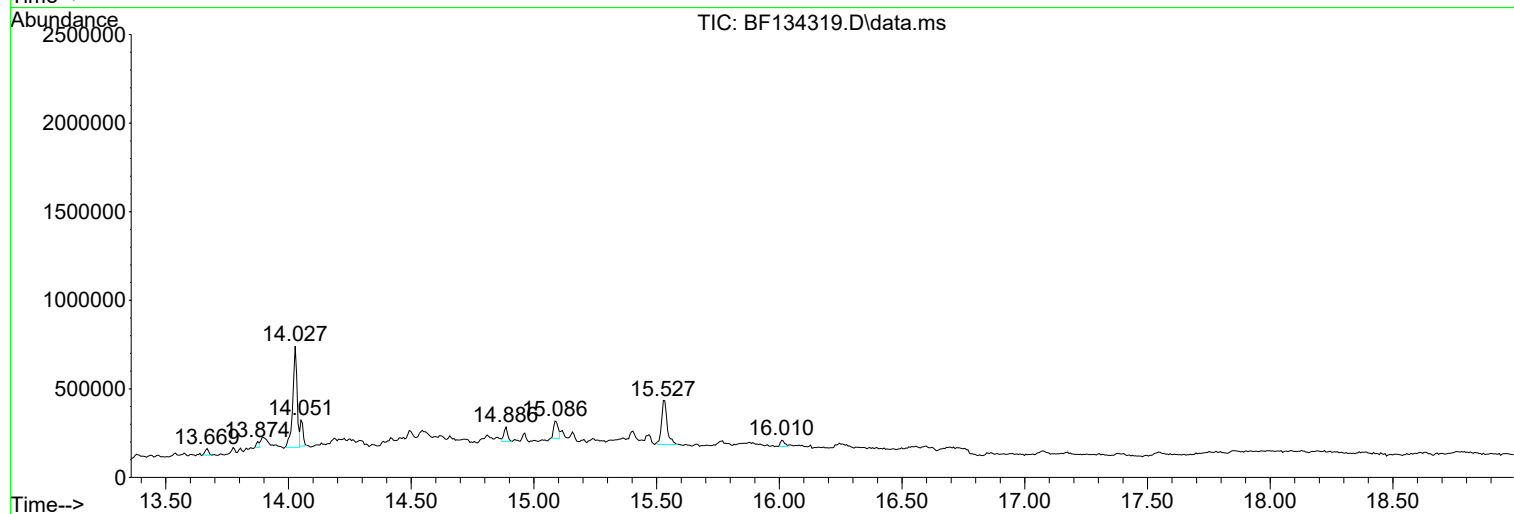
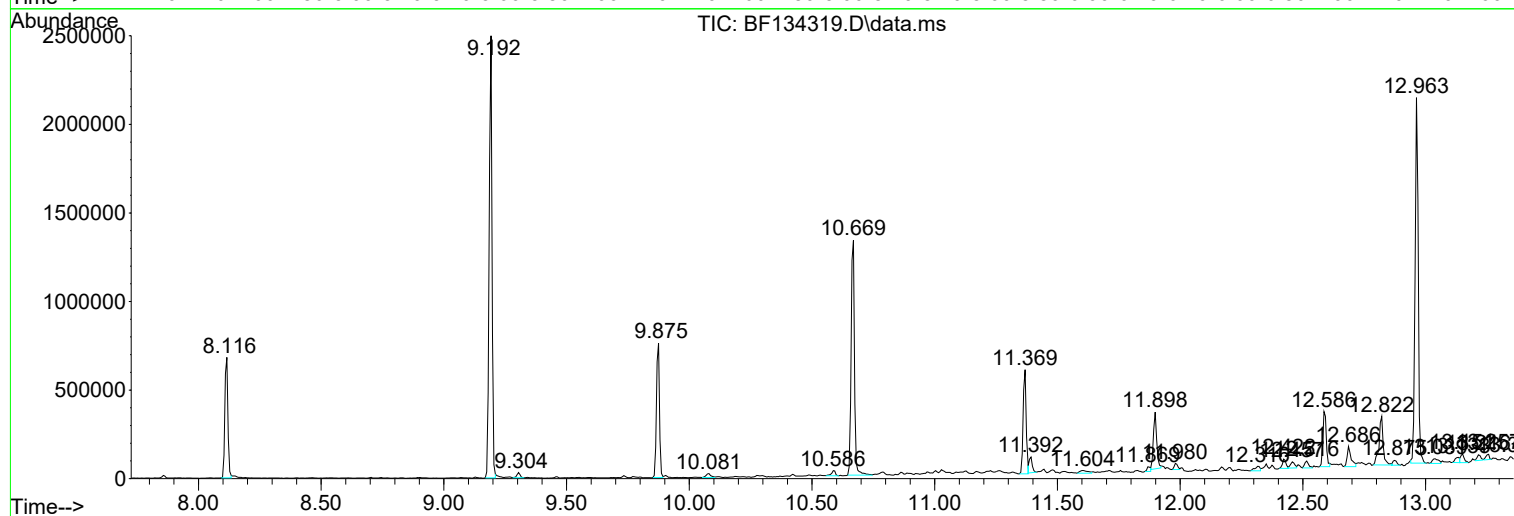
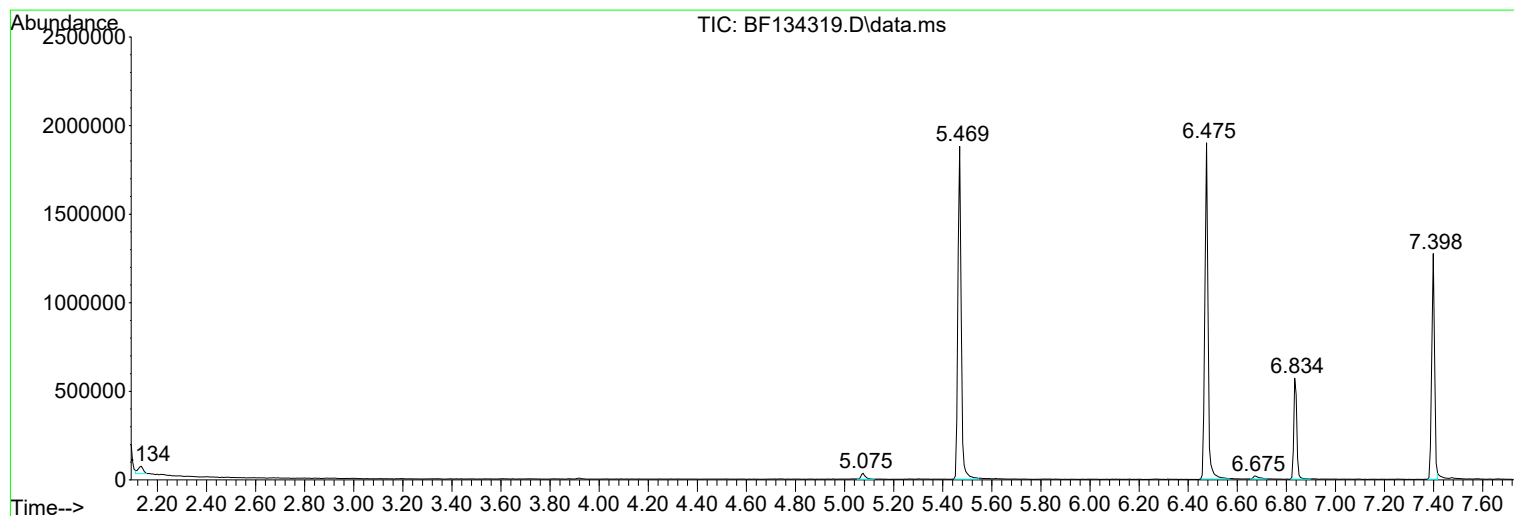
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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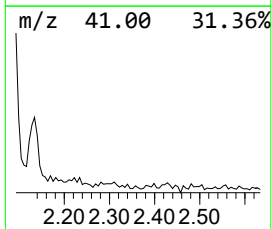
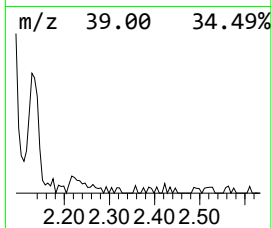
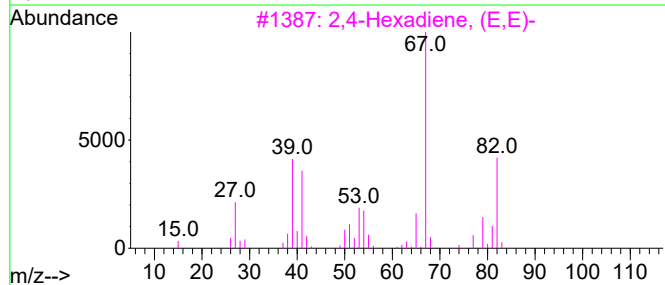
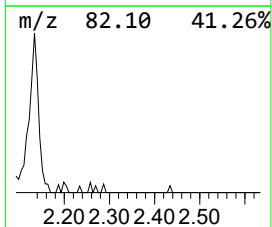
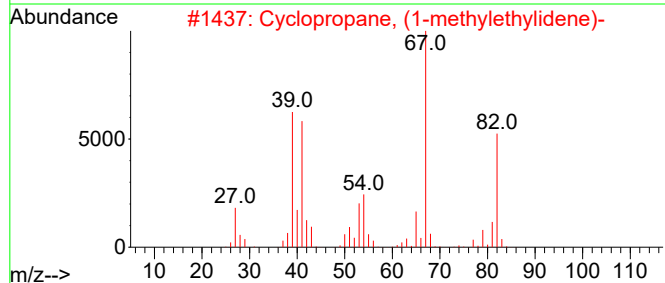
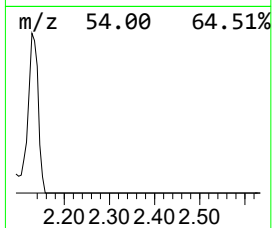
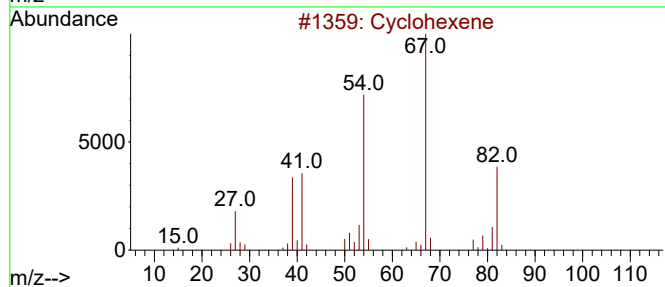
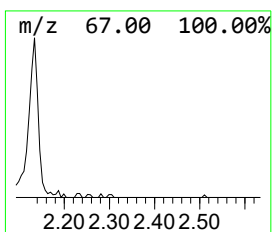
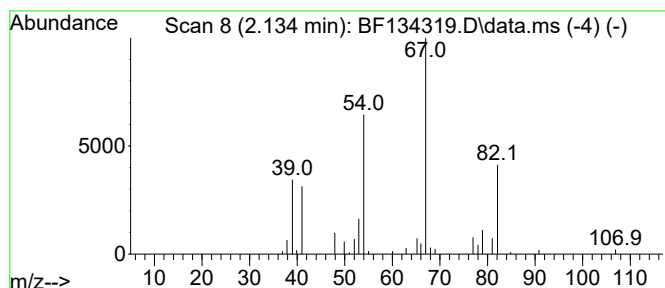
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	2.43 ng	59031	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene	82	C6H10	000110-83-8	64
2			Cyclopropane, (1-methylethylidene)-	82	C6H10	004741-86-0	59
3			2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	58
4			(Z),(Z)-2,4-Hexadiene	82	C6H10	006108-61-8	53
5			1,4-Hexadiene	82	C6H10	000592-45-0	53



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Misc :
ALS Vial : 7 Sample Multiplier: 1

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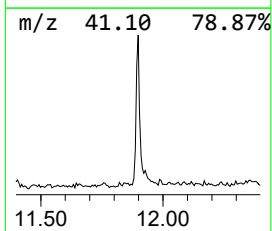
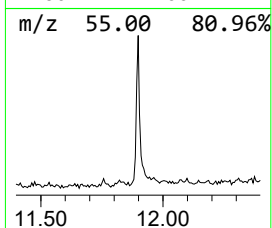
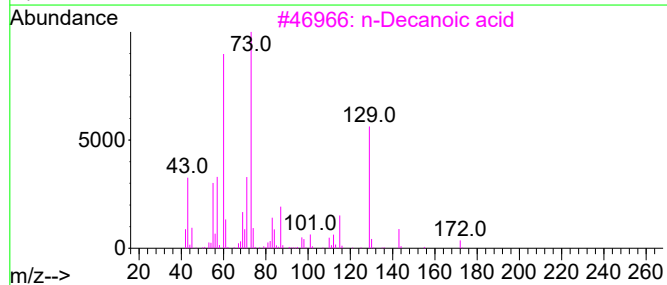
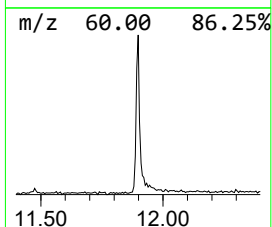
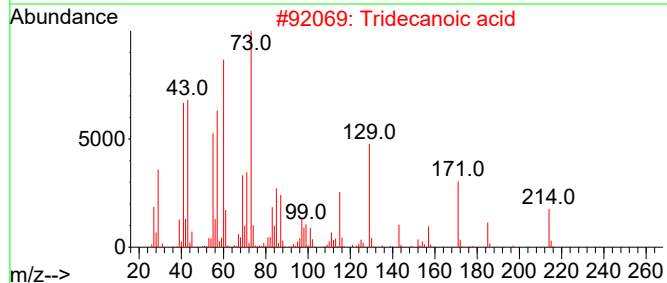
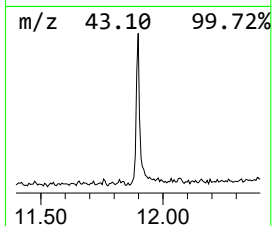
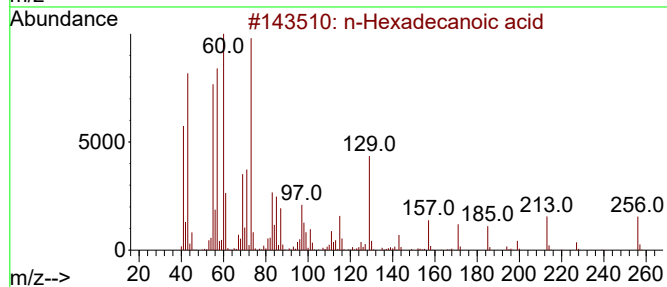
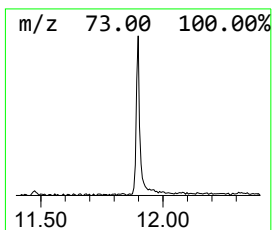
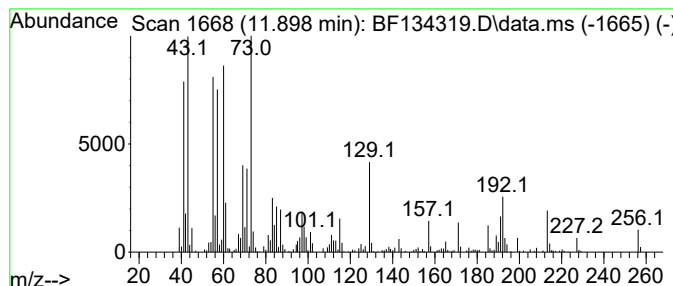
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	11.70 ng	297743	Phenanthrene-d10	11.369

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		n-Decanoic acid	172	C10H20O2	000334-48-5	92
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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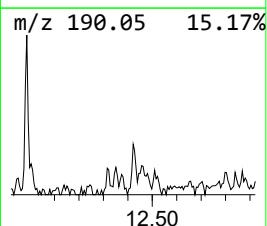
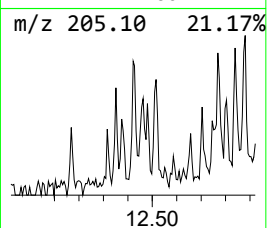
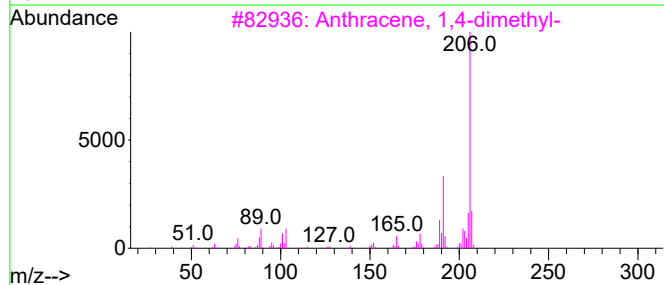
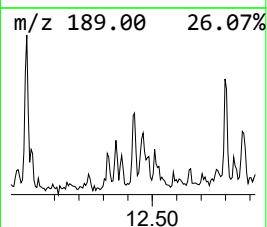
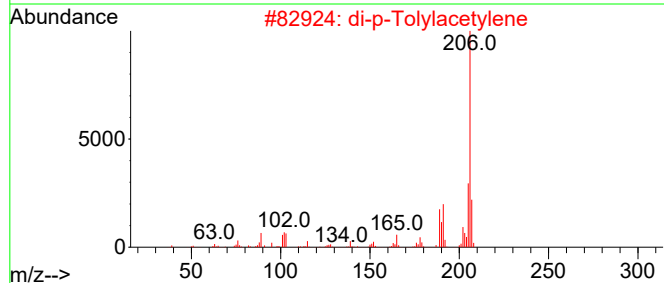
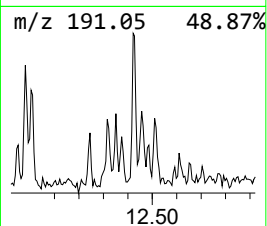
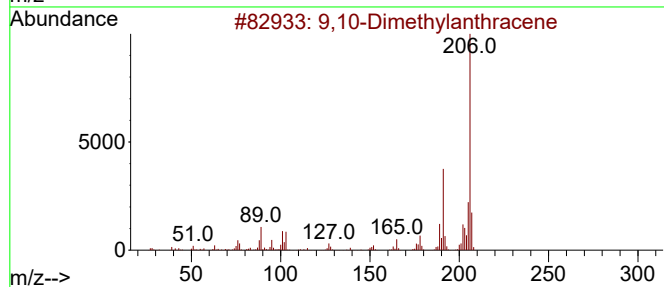
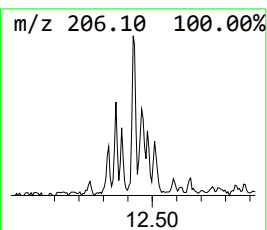
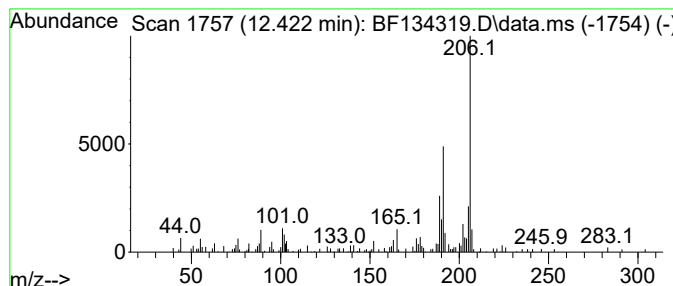
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 9,10-Dimethylantracene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.422	2.03 ng	51760	Phenanthrene-d10		11.369	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylantracene	206	C16H14	000781-43-1	90	
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	83	
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	81	
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	81	
5	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	80	



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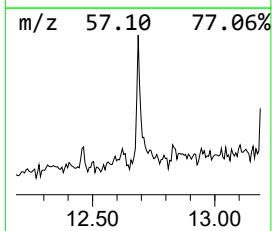
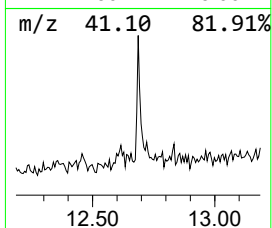
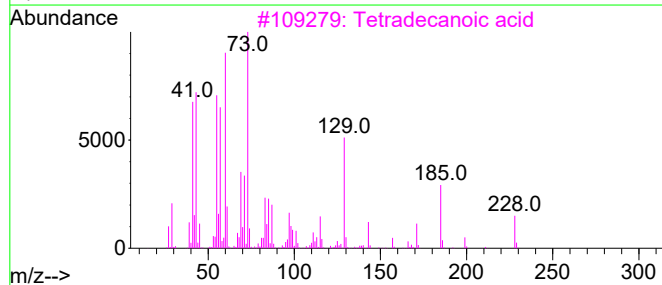
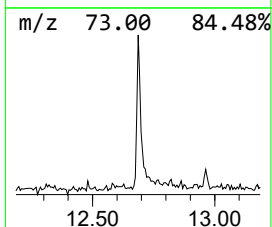
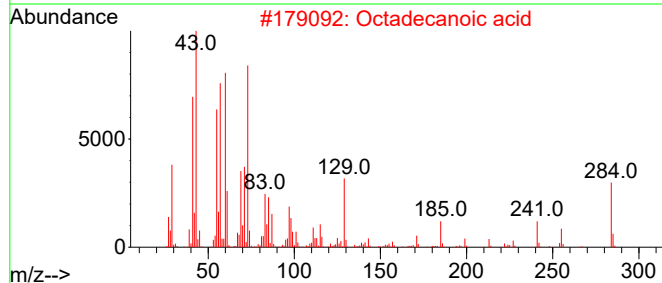
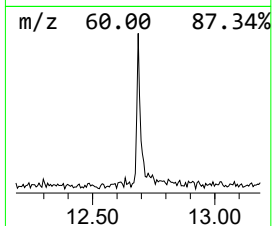
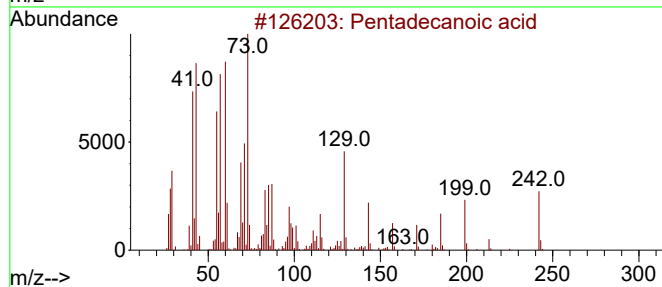
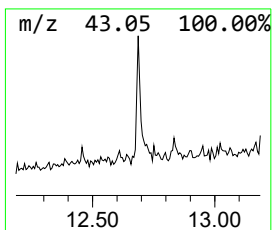
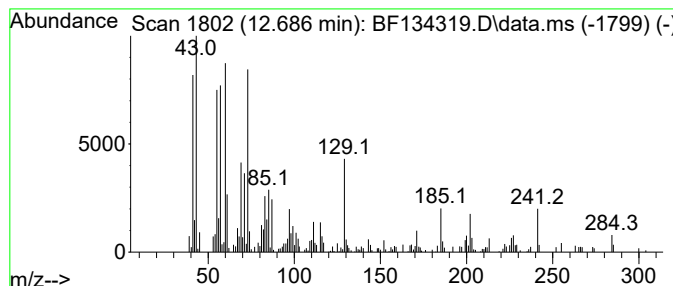
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.686	5.04 ng	128192	Phenanthrene-d10		11.369	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
2	Octadecanoic acid		284	C18H36O2	000057-11-4	80
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
4	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	68
5	Dodecanoic acid		200	C12H24O2	000143-07-7	62



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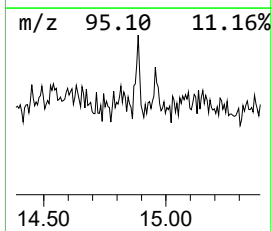
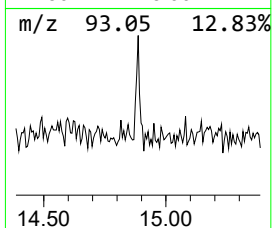
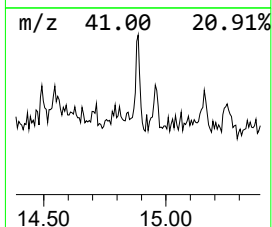
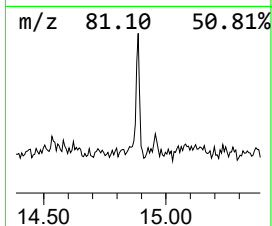
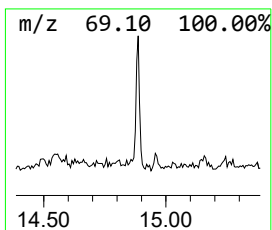
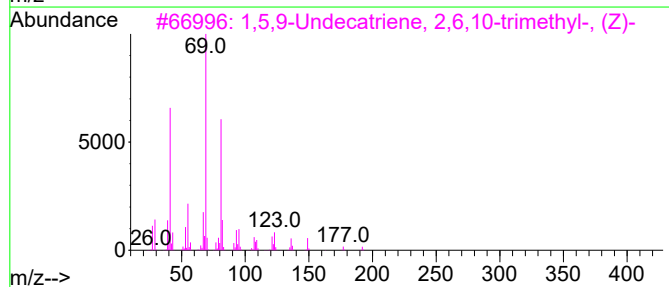
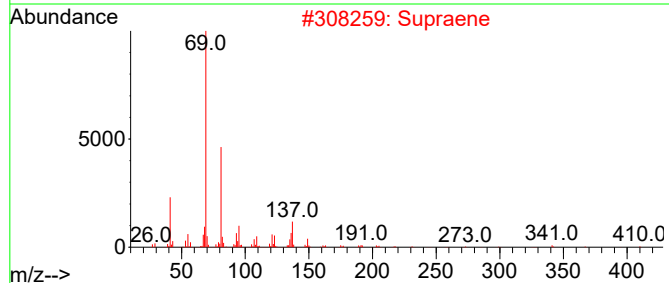
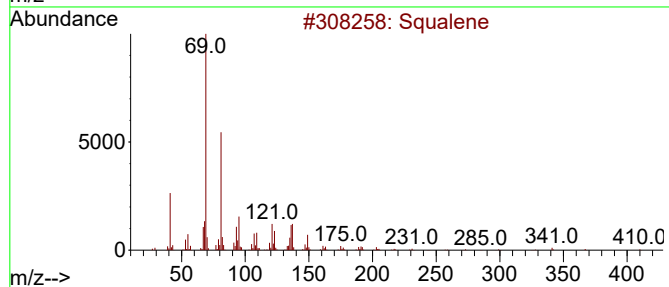
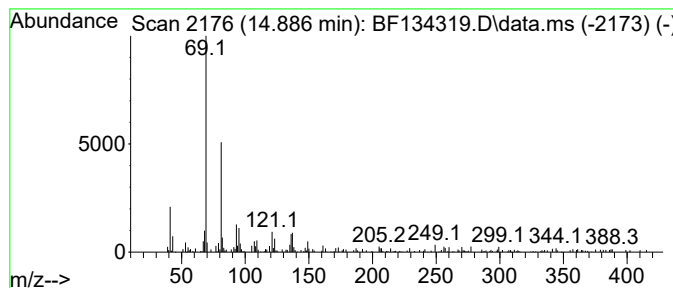
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	4.30 ng	84460	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	87
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134319.D
Acq On : 17 Jul 2023 17:00
Operator : CG\JU
Sample : 03615-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-210

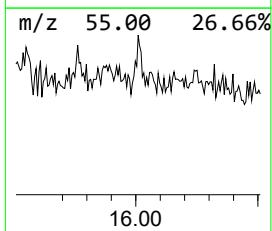
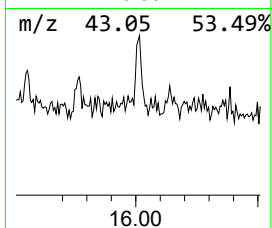
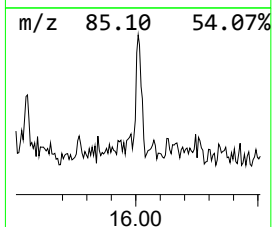
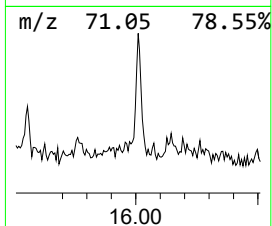
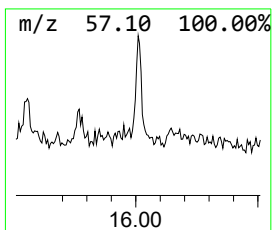
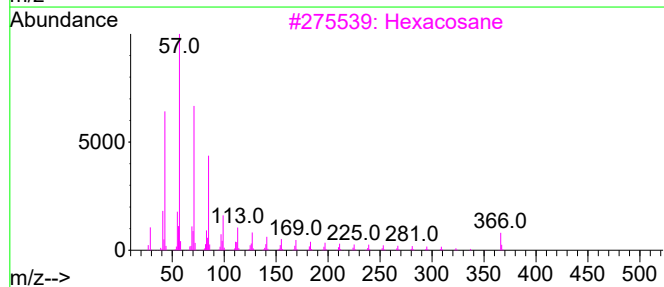
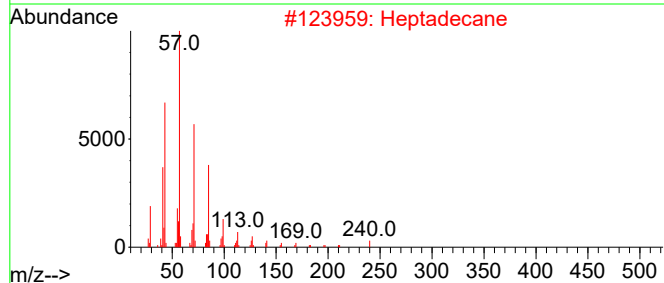
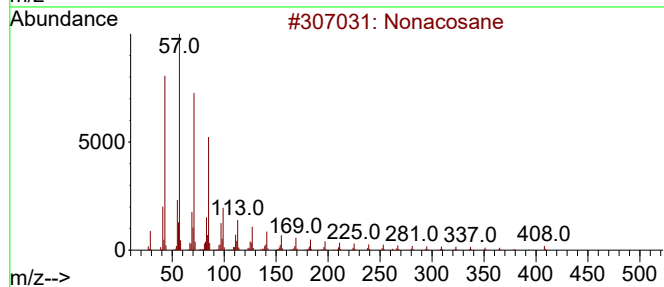
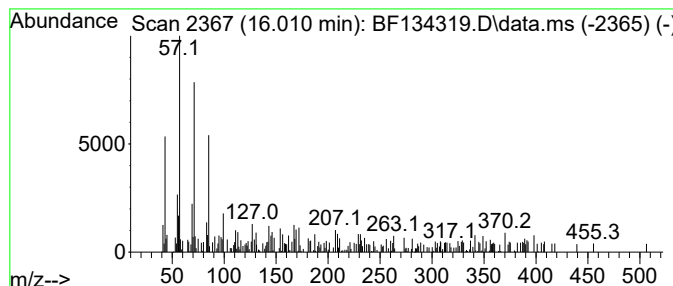
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.010	2.17 ng	42736	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacosane	408	C29H60	000630-03-5	89
2			Heptadecane	240	C17H36	000629-78-7	89
3			Hexacosane	366	C26H54	000630-01-3	76
4			Tetradecane	198	C14H30	000629-59-4	76
5			Heneicosane, 3-methyl-	310	C22H46	006418-47-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071723\
Data File : BF134319.D
Acq On : 17 Jul 2023 17:00
Operator : CG\JU
Sample : 03615-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-210

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexene	2.134	2.4	ng	59031	1	6.834	486838	20.0
n-Hexadecanoic ...	11.898	11.7	ng	297743	4	11.369	509049	20.0
9,10-Dimethylan...	12.422	2.0	ng	51760	4	11.369	509049	20.0
Pentadecanoic acid	12.686	5.0	ng	128192	4	11.369	509049	20.0
Squalene	14.886	4.3	ng	84460	6	15.533	393251	20.0
Nonacosane	16.010	2.2	ng	42736	6	15.533	393251	20.0