

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
 Data File : BF133417.D
 Acq On : 17 May 2023 17:14
 Operator : CG\JU
 Sample : 02812-14
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WG-0516-B4-10-13

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-BF042123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133417.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	474	479	493	rVB	962976	1286112	22.45%	2.979%
2	5.334	547	552	555	rBV	5101321	5195474	90.68%	12.035%
3	5.722	614	618	624	rBV	102079	97420	1.70%	0.226%
4	6.363	722	727	730	rBV	5270060	5214921	91.02%	12.080%
5	6.710	783	786	790	rBV	1563356	1317674	23.00%	3.052%
6	7.281	878	883	886	rBV	4001055	3451877	60.25%	7.996%
7	7.998	1001	1005	1008	rBV	2170376	1759341	30.71%	4.075%
8	9.075	1184	1188	1191	rBV	6512095	5729403	100.00%	13.272%
9	9.751	1299	1303	1306	rBV	2454648	2037751	35.57%	4.720%
10	10.463	1420	1424	1428	rBV	195636	155948	2.72%	0.361%
11	10.539	1433	1437	1452	rBV	3610806	3496533	61.03%	8.099%
12	11.233	1551	1555	1558	rBV	2563707	2104165	36.73%	4.874%
13	11.257	1558	1559	1563	rVB	137031	71896	1.25%	0.167%
14	11.769	1643	1646	1656	rBV3	121301	201613	3.52%	0.467%
15	12.445	1757	1761	1767	rBV	292826	267244	4.66%	0.619%
16	12.669	1792	1799	1802	rBV2	230755	268631	4.69%	0.622%
17	12.822	1821	1825	1828	rBV	5706502	5374259	93.80%	12.449%
18	13.057	1859	1865	1870	rBV2	147420	166739	2.91%	0.386%
19	13.398	1918	1923	1926	rBV2	99053	110662	1.93%	0.256%
20	13.727	1973	1979	1991	rBV2	358732	554170	9.67%	1.284%
21	13.869	1997	2003	2006	rBV	1336944	1309439	22.85%	3.033%
22	13.892	2006	2007	2015	rVB	99474	98314	1.72%	0.228%
23	14.045	2026	2033	2036	rBV	113920	122729	2.14%	0.284%
24	14.351	2081	2085	2087	rBV	155818	190831	3.33%	0.442%
25	14.645	2132	2135	2138	rBV	99651	96841	1.69%	0.224%
26	14.786	2155	2159	2164	rVB2	73223	77778	1.36%	0.180%
27	14.886	2173	2176	2180	rBV	75419	110196	1.92%	0.255%
28	14.968	2186	2190	2193	rBV	150426	156503	2.73%	0.363%
29	15.010	2193	2197	2200	rBV6	39515	74798	1.31%	0.173%
30	15.233	2231	2235	2239	rVB	72830	79185	1.38%	0.183%
31	15.292	2240	2245	2249	rVV	1208162	1414196	24.68%	3.276%
32	15.321	2249	2250	2257	rVB2	107101	124556	2.17%	0.289%
33	15.515	2279	2283	2288	rVB6	41732	64331	1.12%	0.149%
34	15.733	2316	2320	2327	rVB	134696	179653	3.14%	0.416%
35	16.204	2395	2400	2408	rBV3	68416	118929	2.08%	0.275%
36	16.757	2490	2494	2499	rVB	50807	90111	1.57%	0.209%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

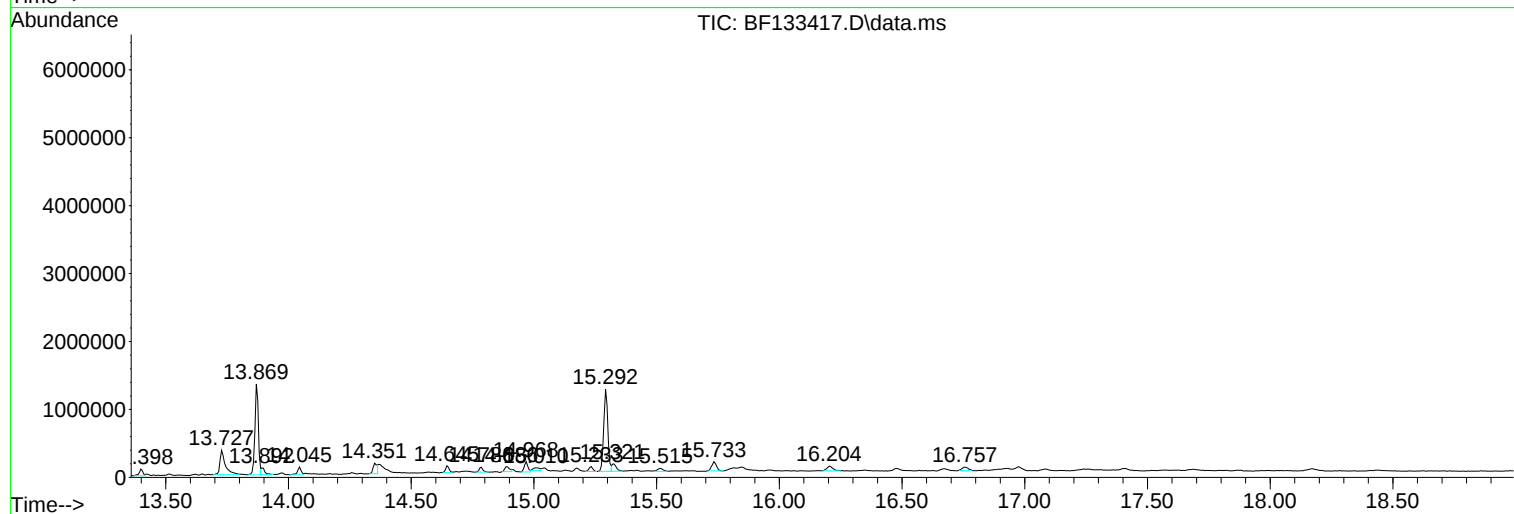
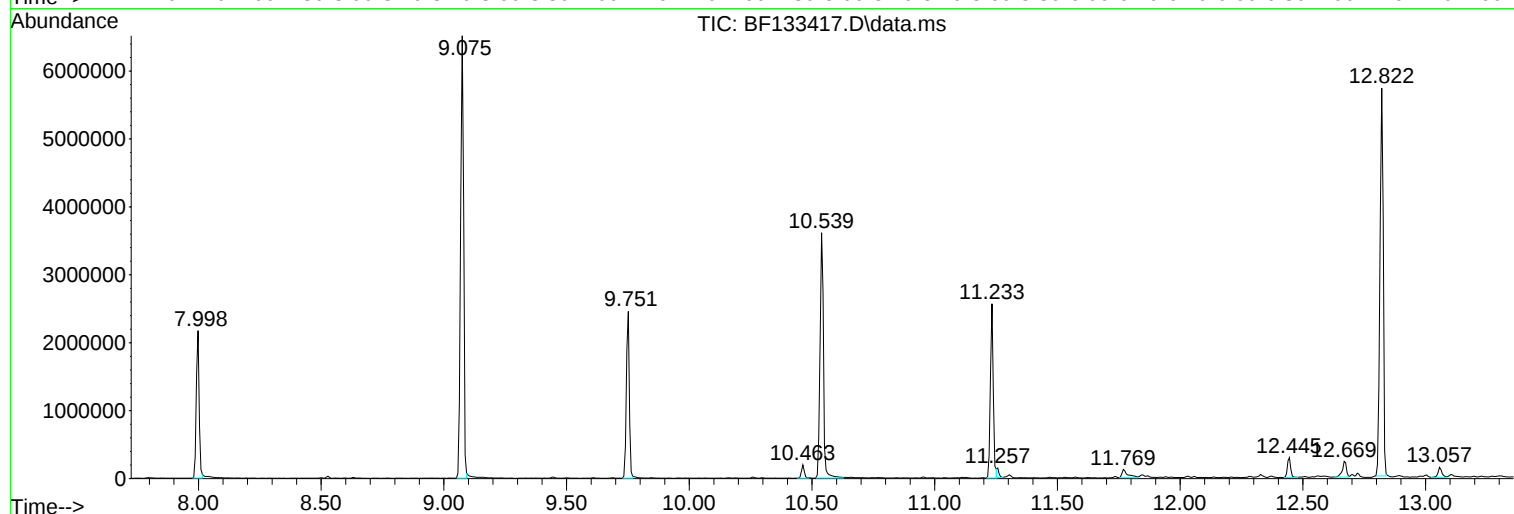
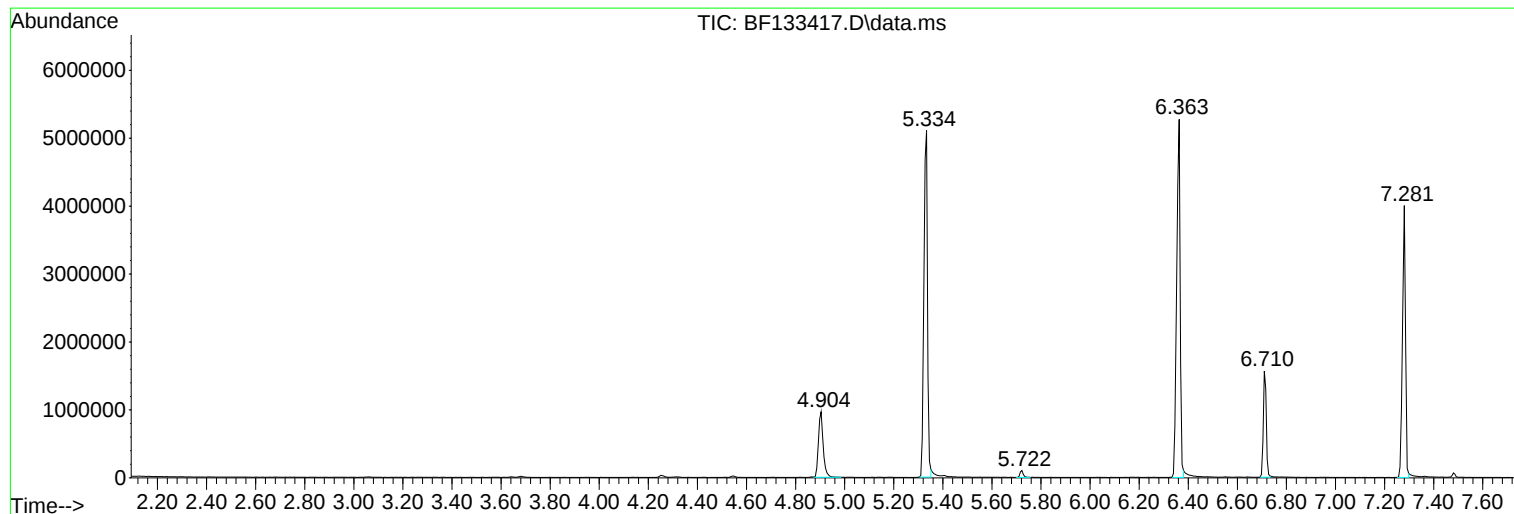
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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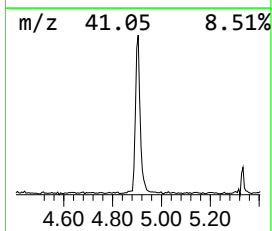
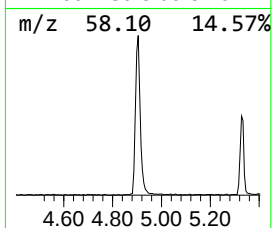
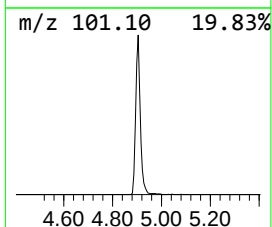
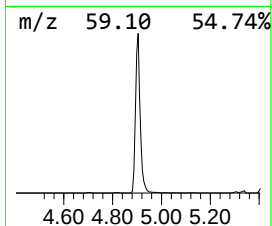
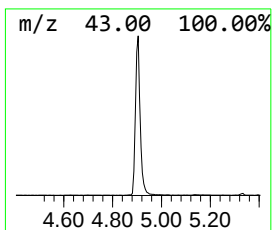
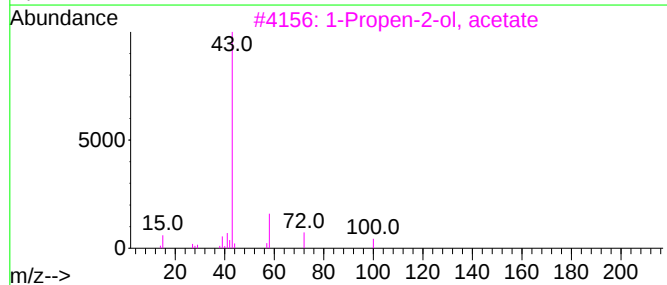
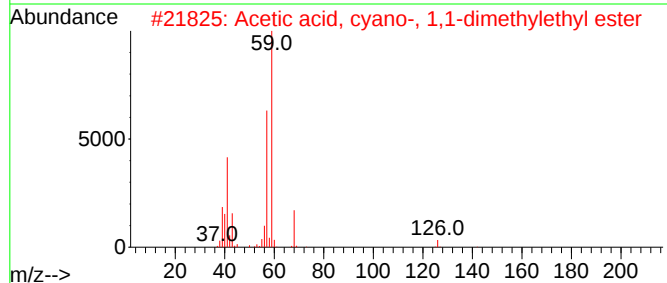
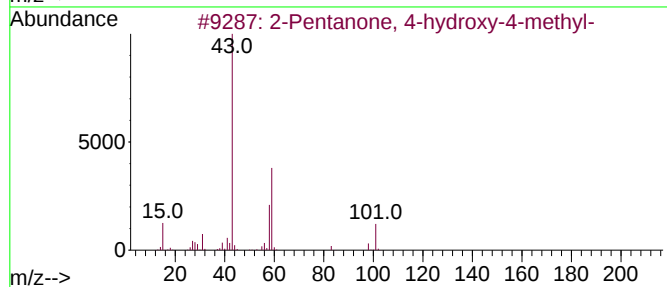
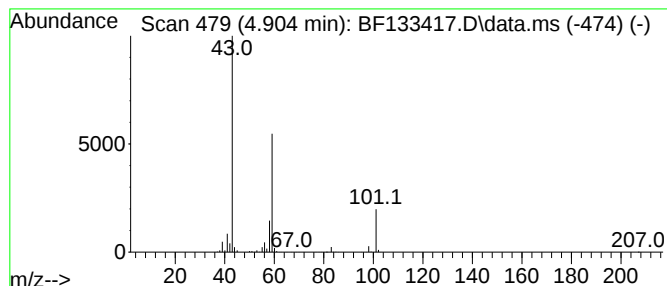
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	19.52 ng	1286110	1,4-Dichlorobenzene-d4	6.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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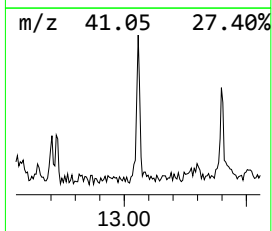
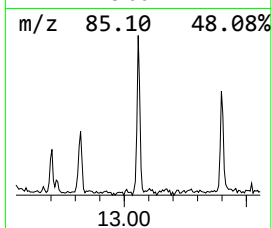
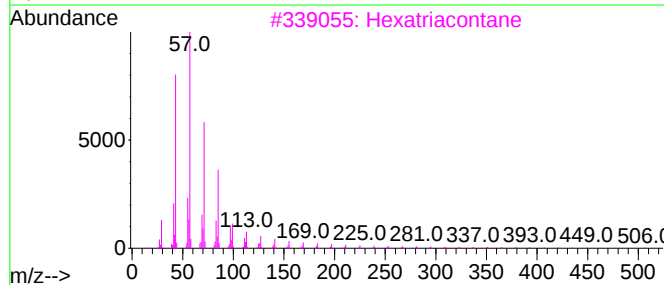
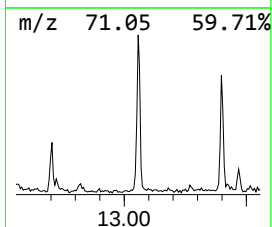
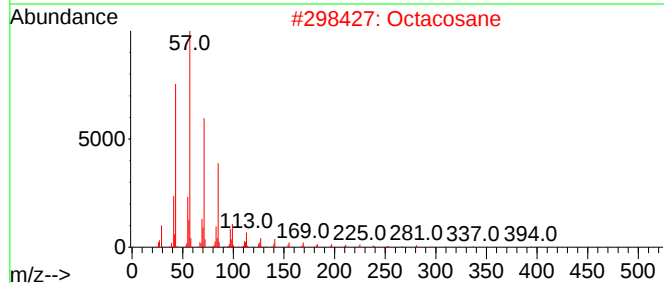
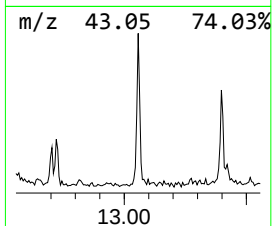
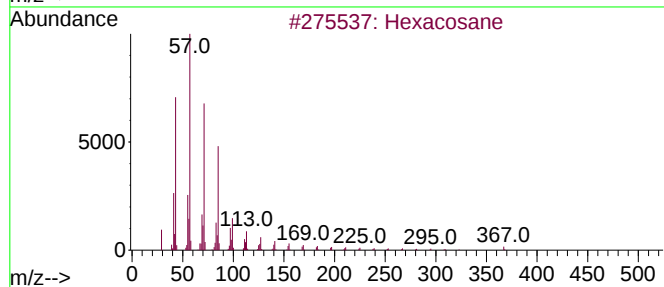
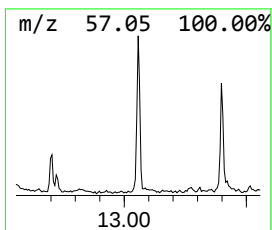
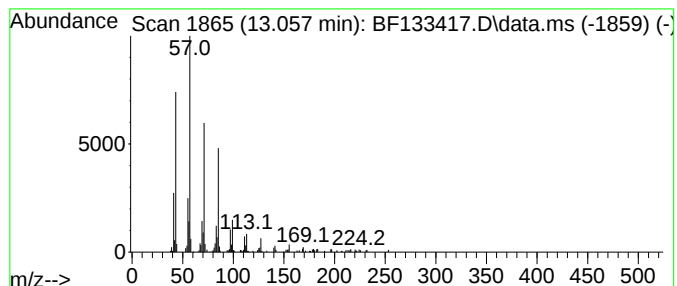
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.057	2.55 ng	166739	Chrysene-d12	13.868

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	93
2		Octacosane	394	C28H58	000630-02-4	90
3		Hexatriacontane	507	C36H74	000630-06-8	90
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5		Heneicosane	296	C21H44	000629-94-7	87



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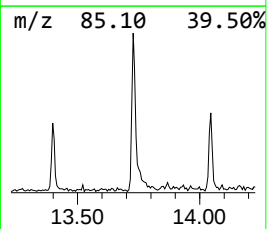
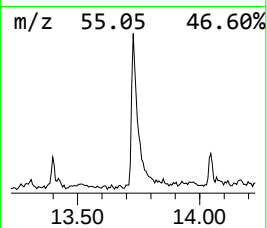
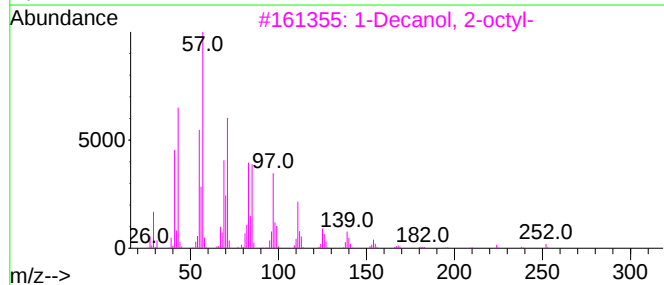
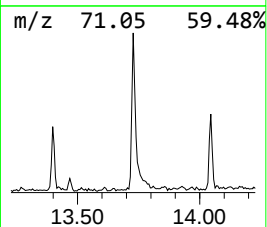
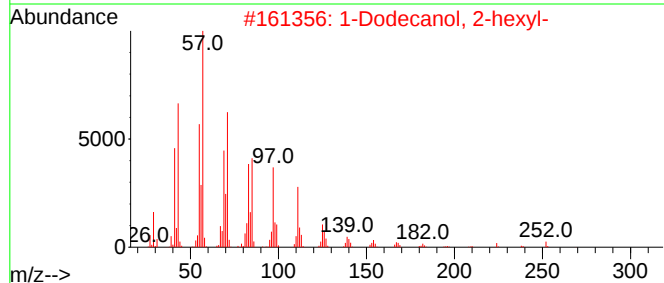
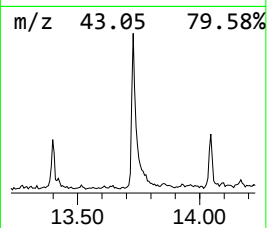
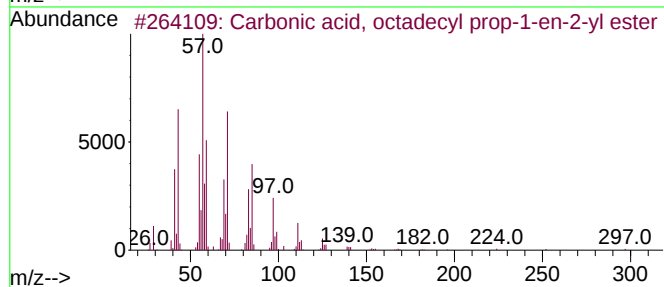
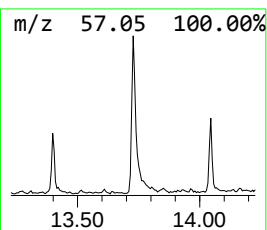
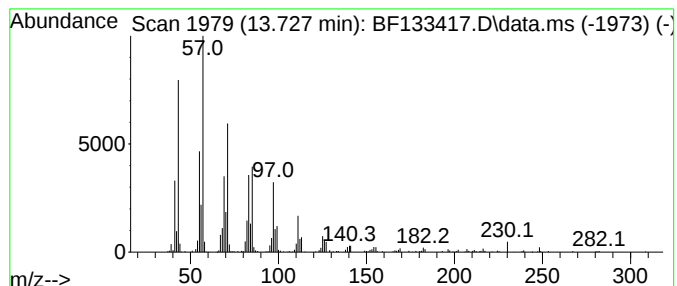
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Carbonic acid, octadecyl pr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	8.46 ng	554170	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
2			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	91
3			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	91
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91



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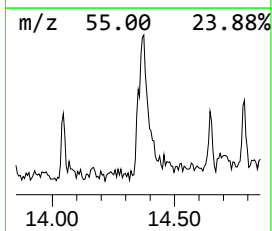
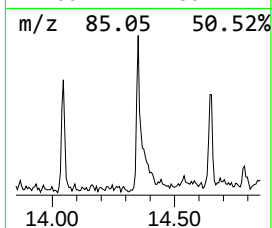
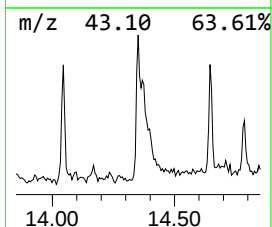
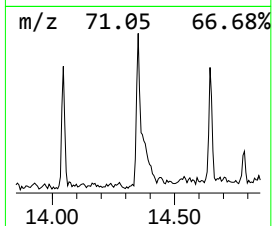
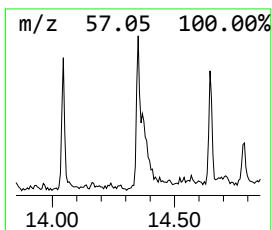
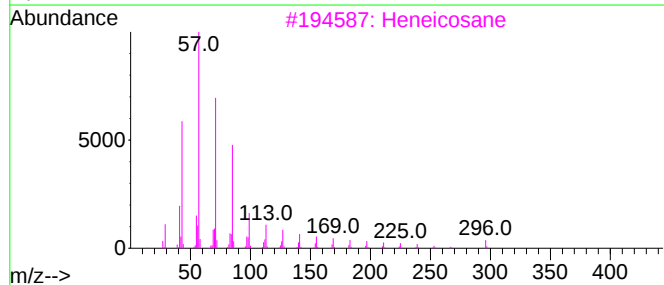
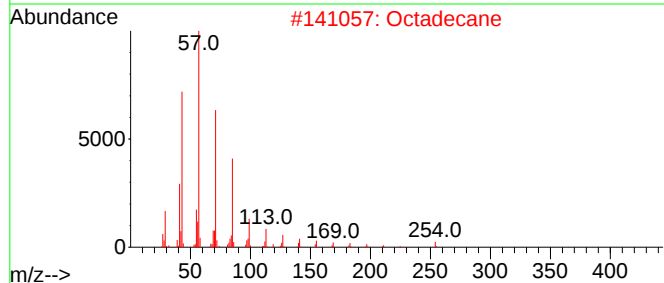
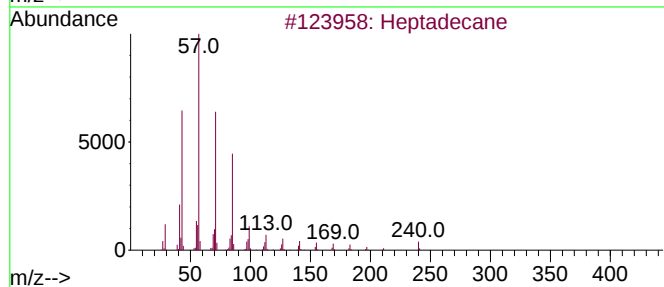
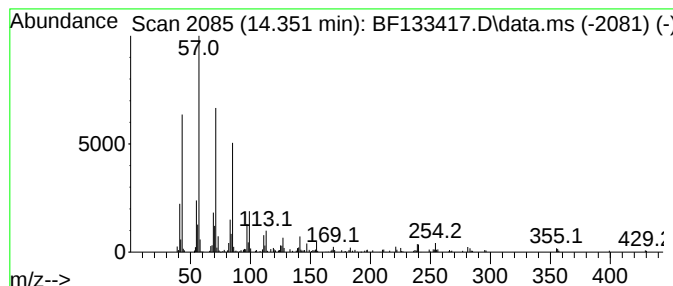
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Peak Number 4 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	2.91 ng	190831	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	98
2			Octadecane	254	C18H38	000593-45-3	97
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



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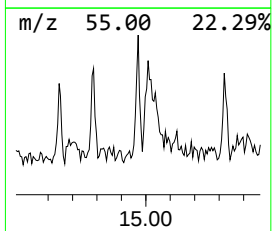
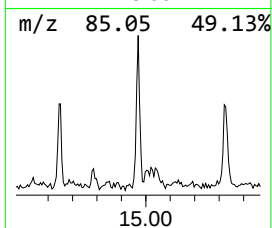
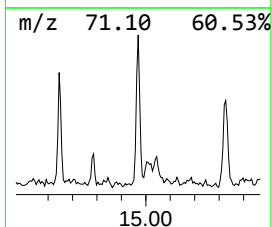
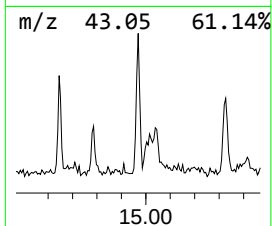
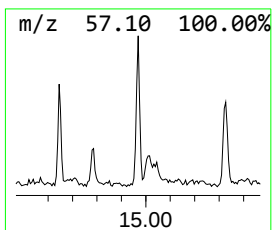
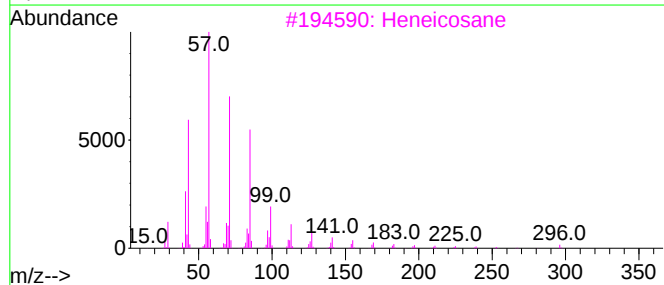
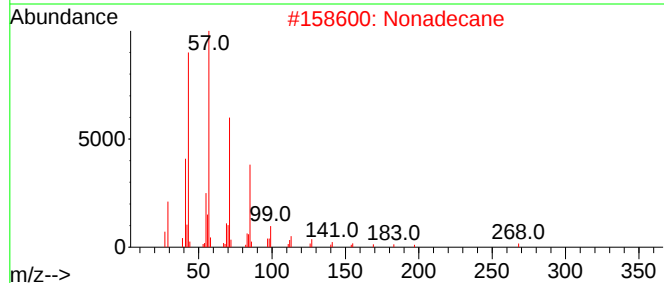
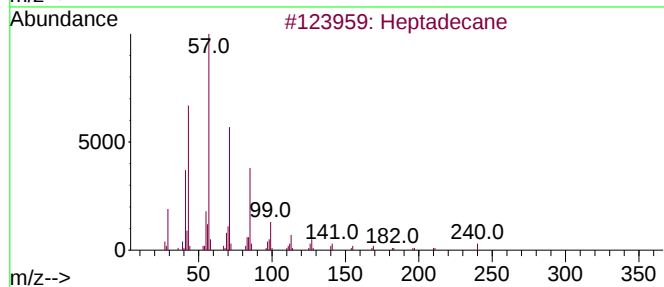
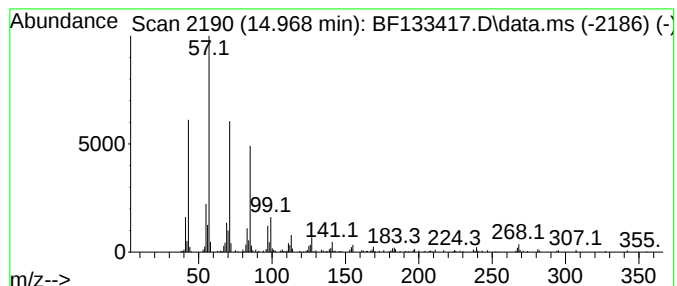
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	2.21 ng	156503	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	95
2			Nonadecane	268	C19H40	000629-92-5	94
3			Heneicosane	296	C21H44	000629-94-7	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133417.D
Acq On : 17 May 2023 17:14
Operator : CG\JU
Sample : 02812-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WG-0516-B4-10-13

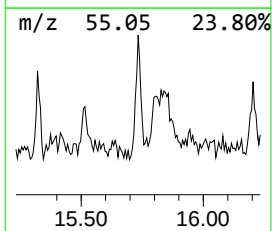
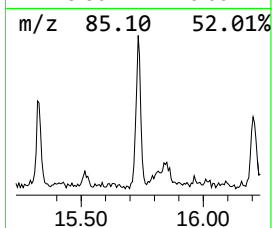
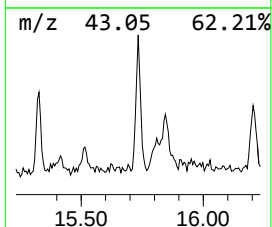
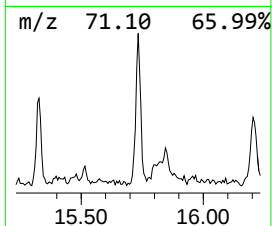
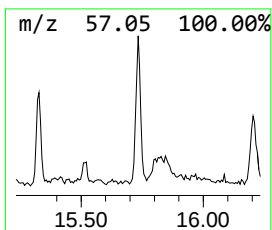
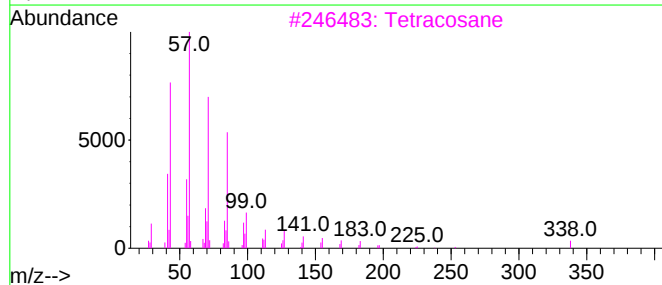
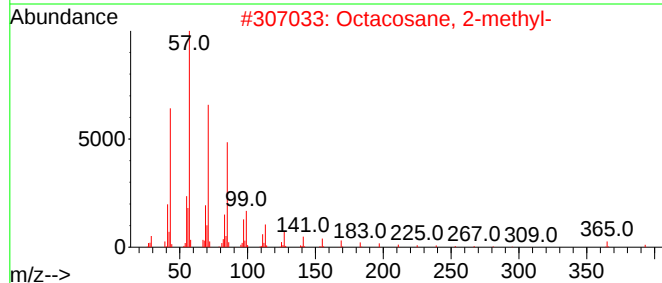
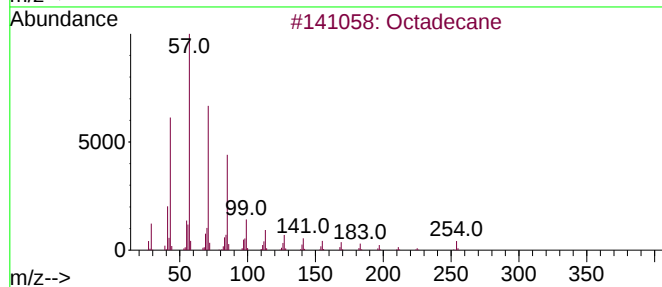
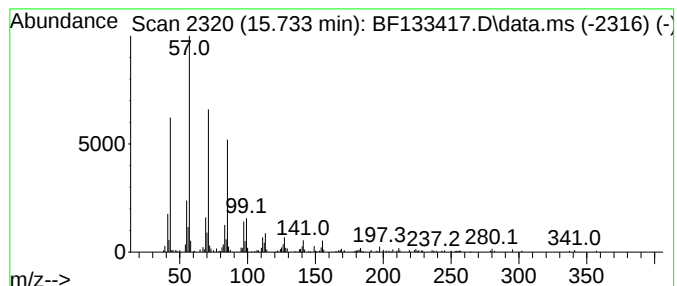
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	2.54 ng	179653	Perylene-d12	15.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	91
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133417.D
Acq On : 17 May 2023 17:14
Operator : CG\JU
Sample : 02812-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WG-0516-B4-10-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
2-Pentanone, 4-...	4.904	19.5	ng	1286110	1	6.710	1317670	20.0
Hexacosane	13.057	2.5	ng	166739	5	13.868	1309440	20.0
Carbonic acid, ...	13.727	8.5	ng	554170	5	13.868	1309440	20.0
Heptadecane	14.351	2.9	ng	190831	5	13.868	1309440	20.0
Nonadecane	14.968	2.2	ng	156503	6	15.292	1414200	20.0
Octadecane	15.733	2.5	ng	179653	6	15.292	1414200	20.0