

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
 Data File : BF133876.D
 Acq On : 21 Jun 2023 17:57
 Operator : CG\JU
 Sample : 03296-19
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSIT-TW-07

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-BF060923.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133876.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	7	12	18	rVB	502641	634633	20.25%	2.840%
2	2.275	28	32	40	rVB2	29429	53337	1.70%	0.239%
3	5.098	507	512	523	rVB	781210	985063	31.44%	4.408%
4	5.498	575	580	583	rBV	2267551	2045864	65.29%	9.154%
5	5.881	642	645	650	rBV	57448	48285	1.54%	0.216%
6	6.498	745	750	753	rBV	2163961	2034869	64.94%	9.105%
7	6.857	808	811	815	rBV	723716	602662	19.23%	2.697%
8	7.422	902	907	910	rBV	1601595	1321000	42.16%	5.911%
9	8.139	1025	1029	1032	rBV	904344	703091	22.44%	3.146%
10	9.216	1208	1212	1215	rBV	2850092	2227283	71.08%	9.966%
11	9.898	1324	1328	1331	rBV	750098	624145	19.92%	2.793%
12	10.610	1445	1449	1453	rBV	107945	91658	2.92%	0.410%
13	10.686	1458	1462	1474	rBV	1255558	1098549	35.06%	4.916%
14	11.392	1578	1582	1584	rBV	629419	581714	18.56%	2.603%
15	11.410	1584	1585	1589	rVV	186297	151243	4.83%	0.677%
16	11.463	1592	1594	1597	rVB	52913	43561	1.39%	0.195%
17	11.621	1615	1621	1627	rBV2	23696	33714	1.08%	0.151%
18	11.886	1662	1666	1669	rBV2	239716	243102	7.76%	1.088%
19	11.921	1669	1672	1683	rVB	499461	487163	15.55%	2.180%
20	12.004	1683	1686	1689	rBV	50531	54789	1.75%	0.245%
21	12.445	1758	1761	1765	rBV2	26462	31590	1.01%	0.141%
22	12.533	1773	1776	1781	rBV2	25659	35194	1.12%	0.157%
23	12.610	1785	1789	1792	rVV	551708	478293	15.26%	2.140%
24	12.645	1793	1795	1803	rVB4	74167	101678	3.24%	0.455%
25	12.710	1803	1806	1811	rBV2	83744	93154	2.97%	0.417%
26	12.839	1822	1828	1833	rBV	495333	511230	16.31%	2.288%
27	12.986	1849	1853	1856	rBV	2141861	1808529	57.71%	8.092%
28	13.057	1861	1865	1870	rBV4	37645	62384	1.99%	0.279%
29	13.168	1882	1884	1888	rVB	62514	60709	1.94%	0.272%
30	13.215	1888	1892	1894	rBV3	35051	48773	1.56%	0.218%
31	13.239	1894	1896	1898	rVV	47786	36318	1.16%	0.163%
32	13.274	1899	1902	1905	rVB2	43542	47616	1.52%	0.213%
33	13.463	1932	1934	1940	rVB3	34982	36743	1.17%	0.164%
34	13.680	1969	1971	1977	rVB2	49193	49223	1.57%	0.220%
35	13.845	1997	1999	2001	rBV	32783	32439	1.04%	0.145%
36	13.892	2004	2007	2014	rVV3	172871	240912	7.69%	1.078%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.033	2026	2031	2036	rBV2	2711706	3133616	100.00%	14.022%
38	14.074	2036	2038	2044	rVB	243807	213165	6.80%	0.954%
39	14.151	2049	2051	2054	rVB2	50571	45407	1.45%	0.203%
40	14.521	2112	2114	2115	rBV	52518	43307	1.38%	0.194%
41	14.992	2191	2194	2197	rBV	119099	117735	3.76%	0.527%
42	15.109	2211	2214	2218	rBV	188254	267982	8.55%	1.199%
43	15.192	2225	2228	2231	rVB	103418	98256	3.14%	0.440%
44	15.492	2276	2279	2285	rVB	138978	183669	5.86%	0.822%
45	15.556	2286	2290	2294	rBV	273370	356366	11.37%	1.595%
46	16.062	2373	2376	2382	rVB2	106553	148528	4.74%	0.665%

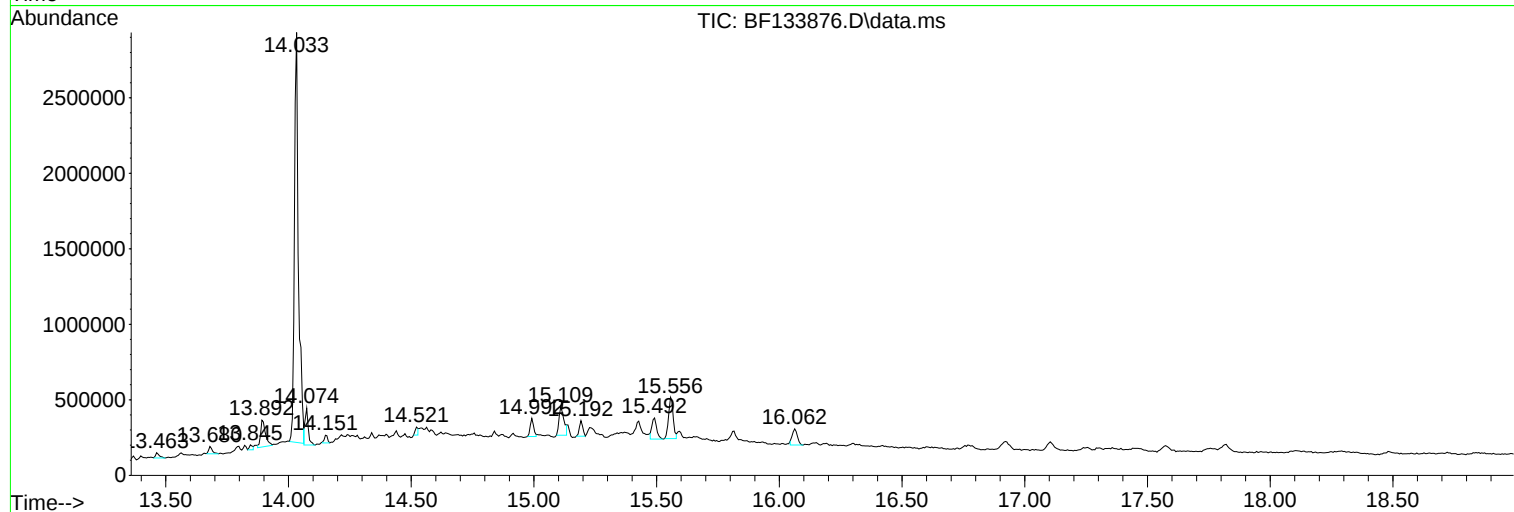
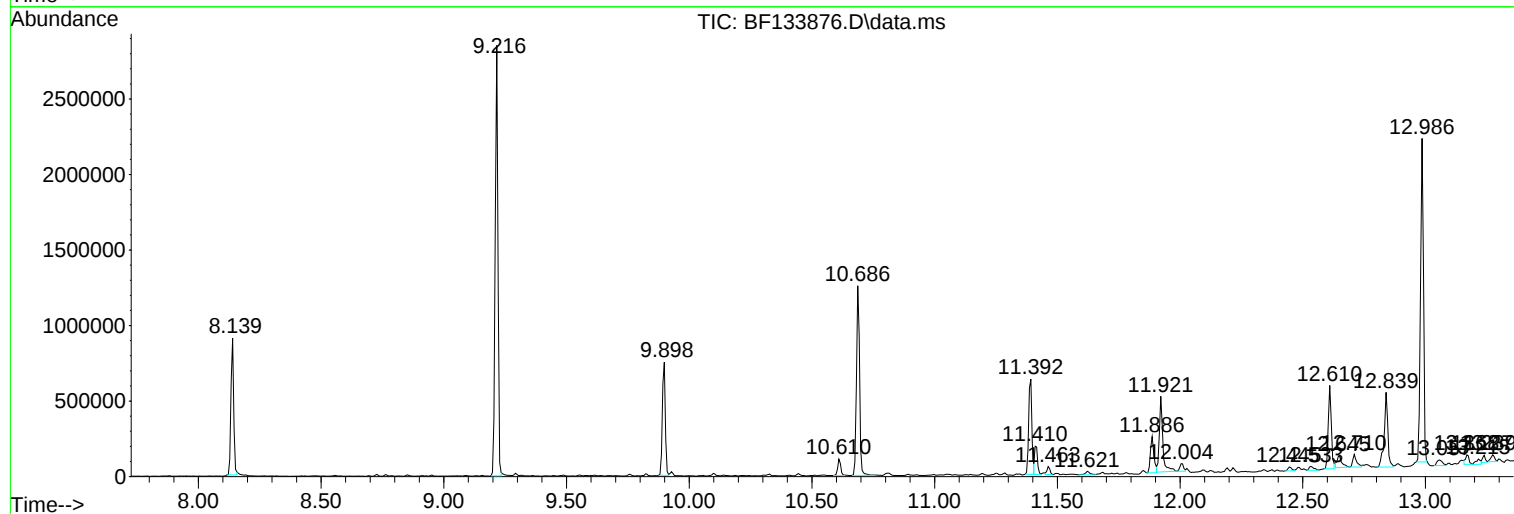
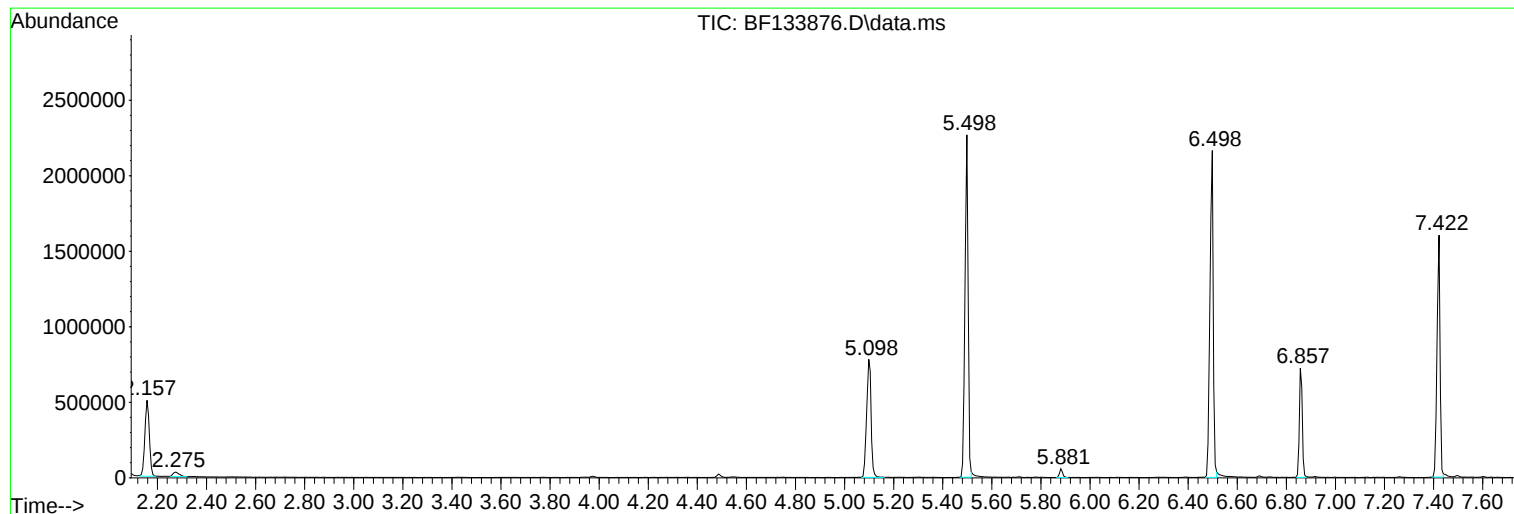
Sum of corrected areas: 22348541

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

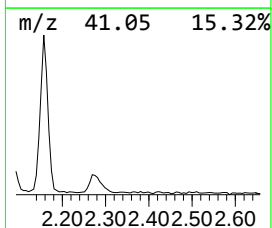
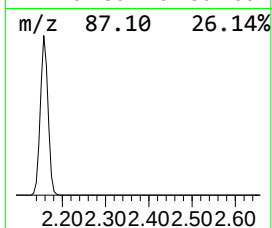
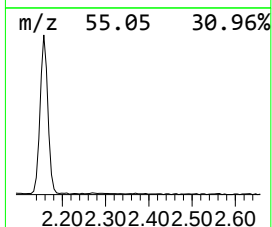
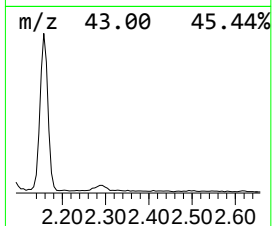
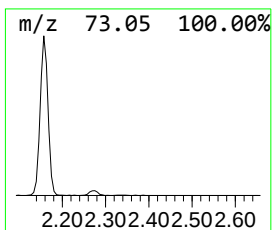
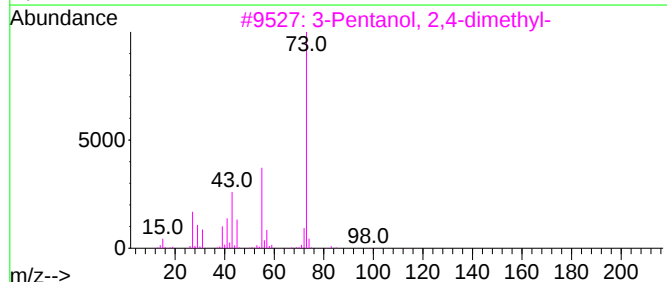
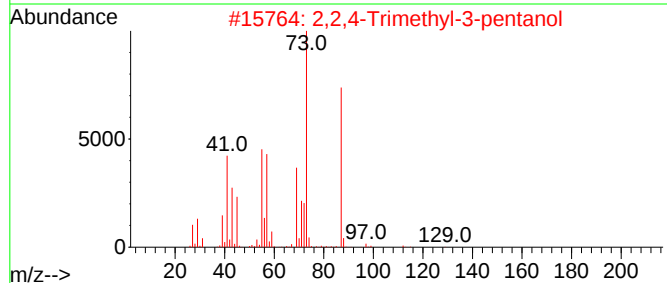
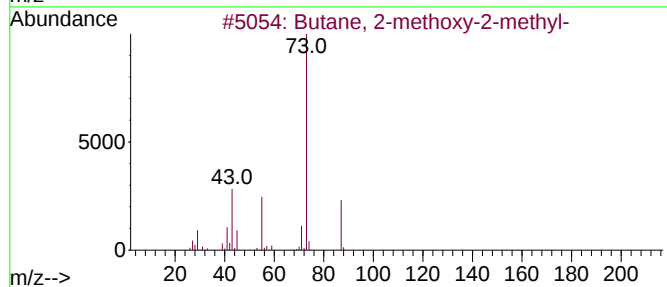
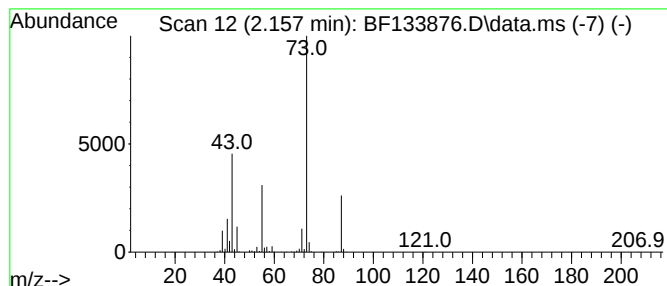
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	21.06 ng	634633	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

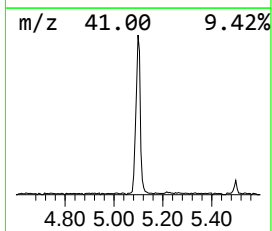
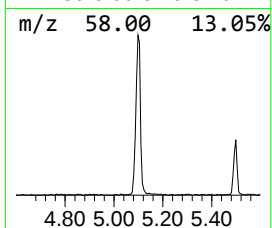
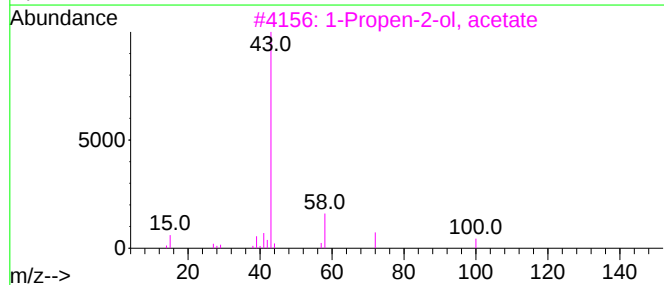
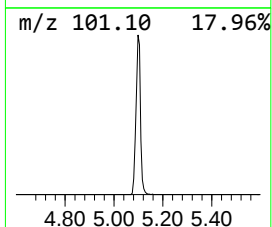
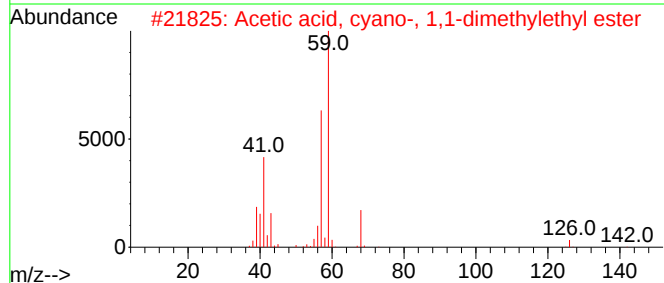
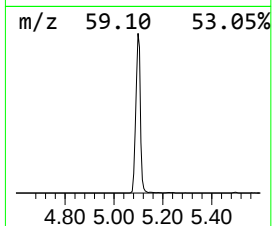
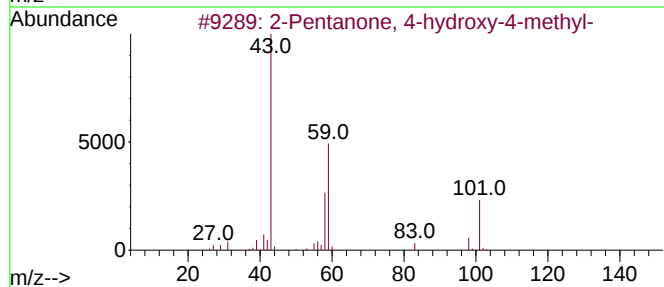
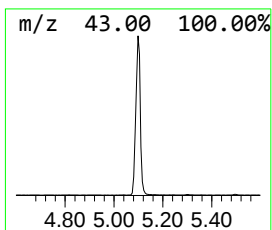
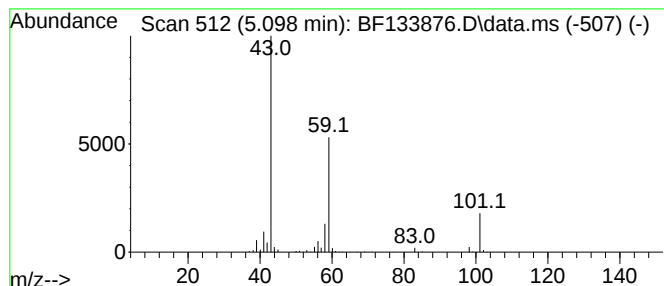
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	32.69 ng	985063	1,4-Dichlorobenzene-d4	6.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

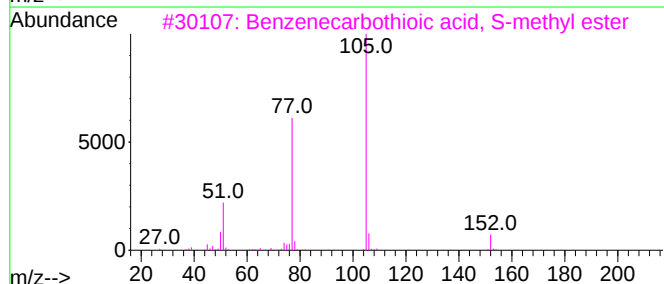
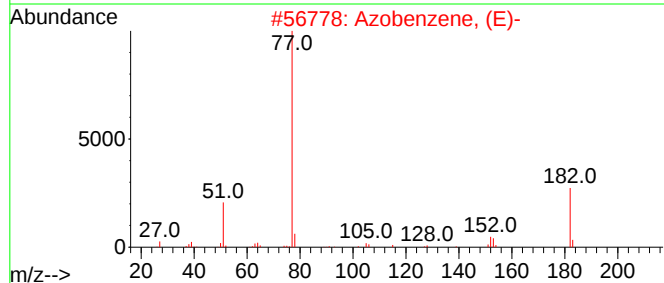
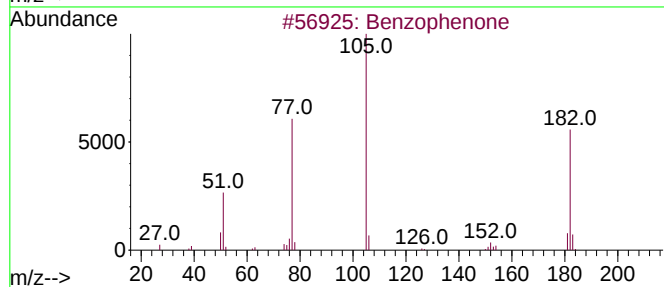
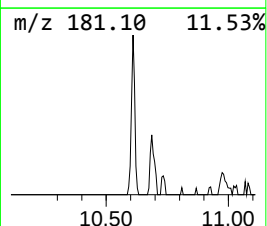
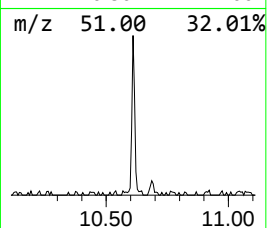
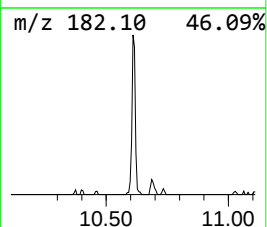
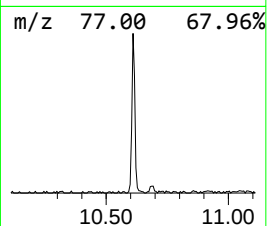
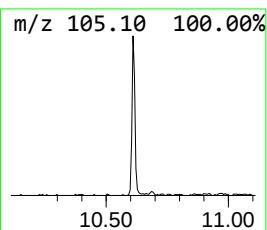
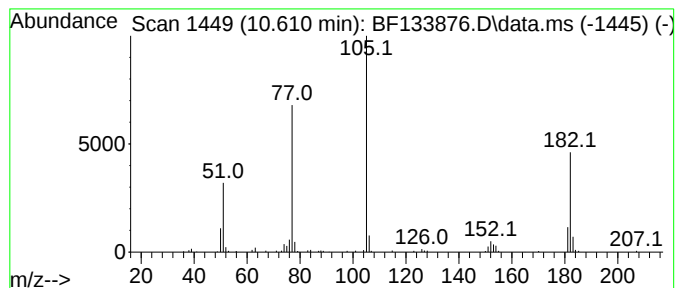
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	2.94 ng	91658	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
5			Benzoylformic acid	150	C8H6O3	000611-73-4	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

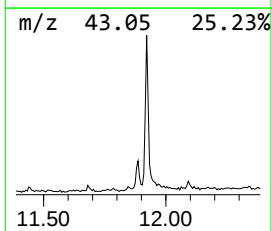
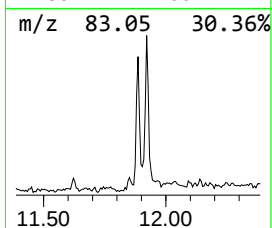
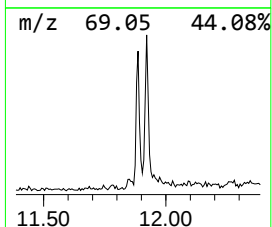
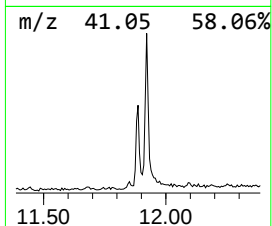
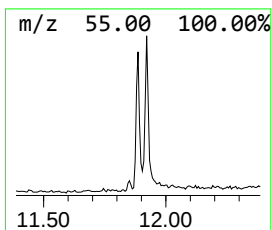
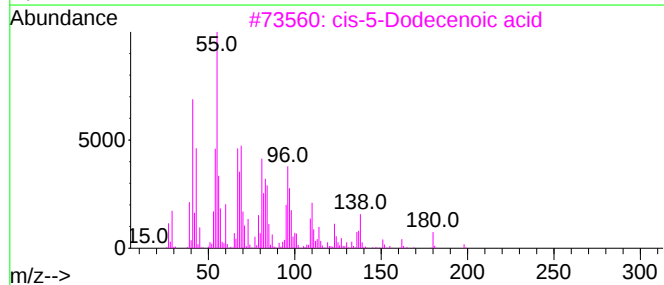
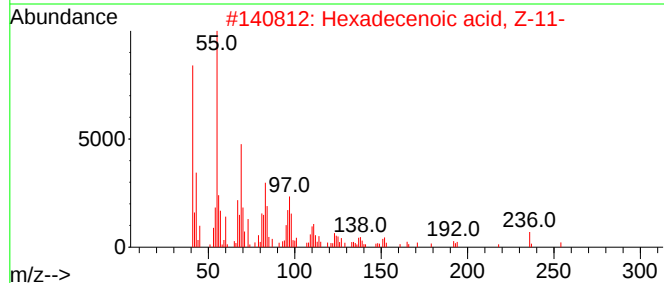
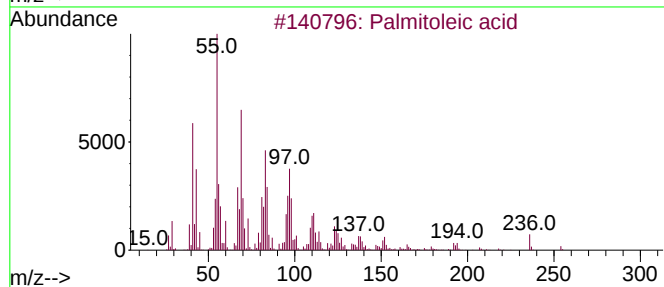
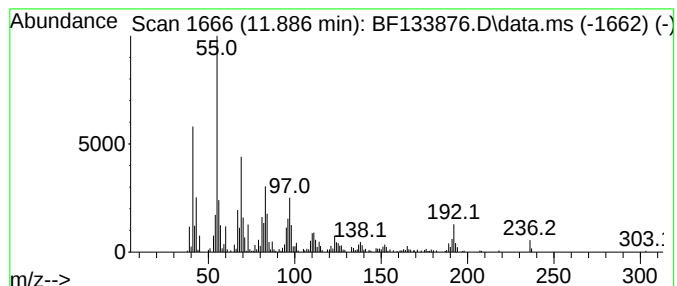
Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Palmitoleic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.886	8.36 ng	243102	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleic acid	254	C16H30O2	000373-49-9	90
2	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	90
3	cis-5-Dodecenoic acid	198	C12H22O2	002430-94-6	89
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
5	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

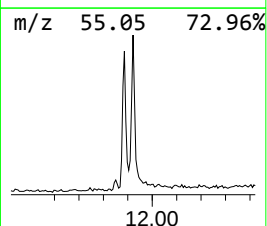
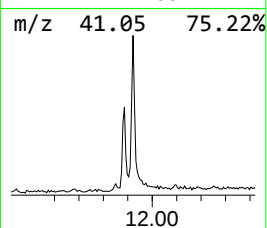
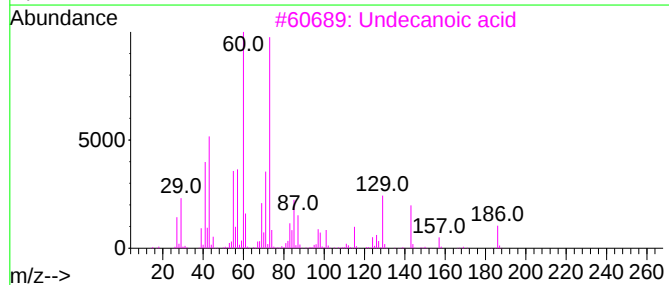
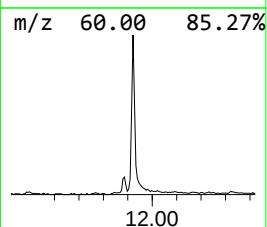
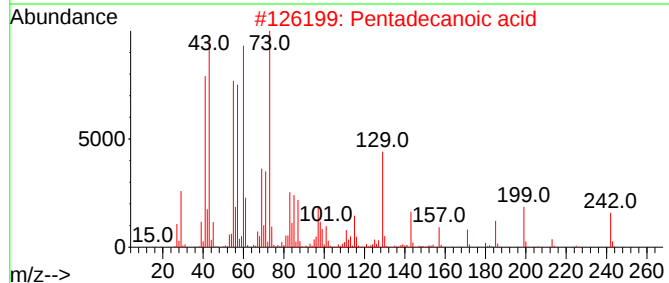
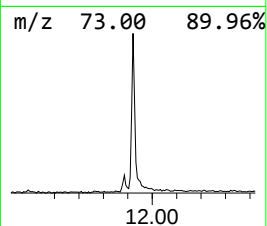
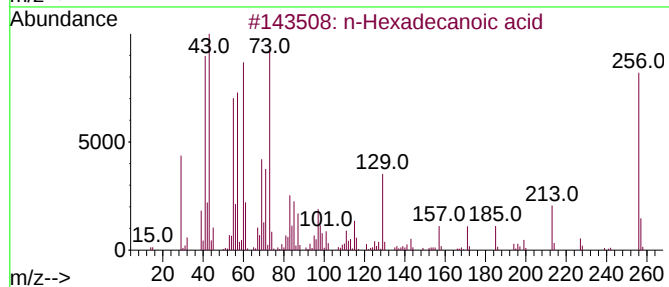
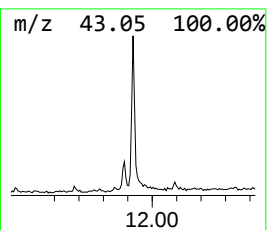
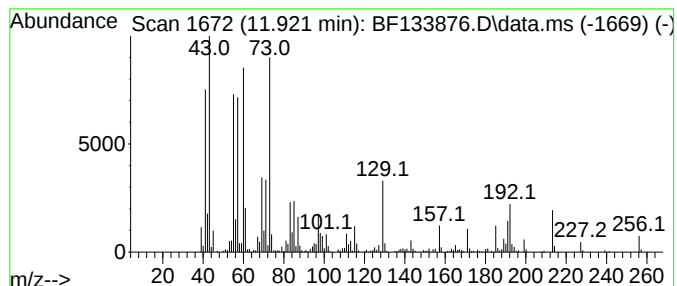
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.921	16.75 ng	487163	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3			Undecanoic acid	186	C11H22O2	000112-37-8	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

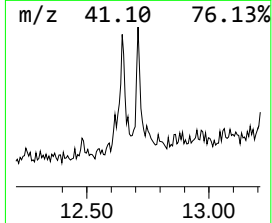
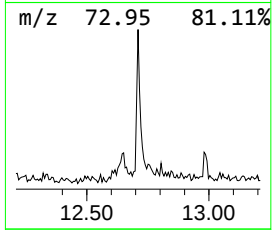
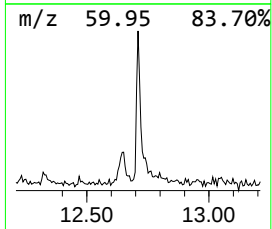
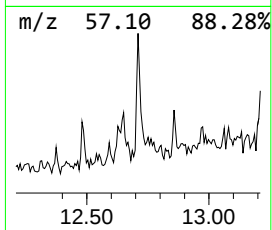
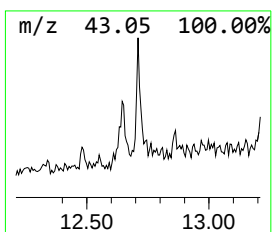
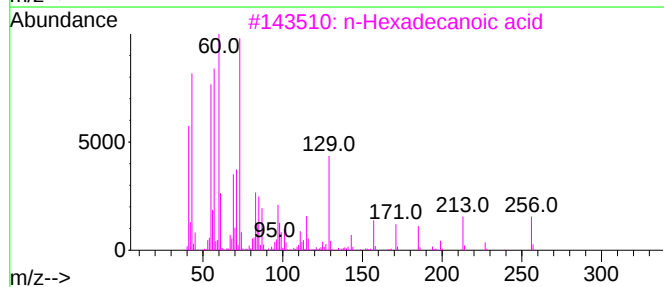
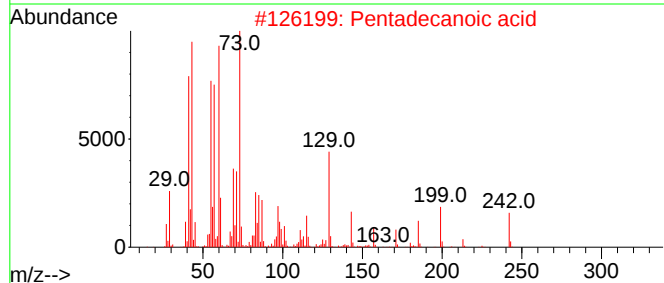
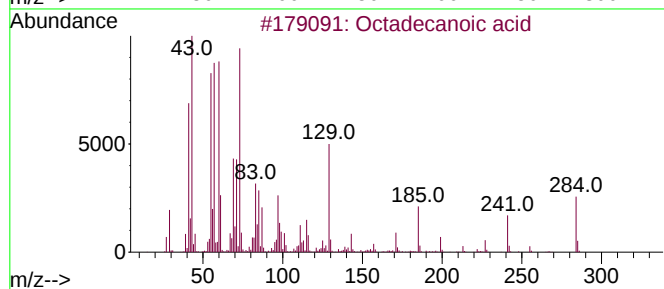
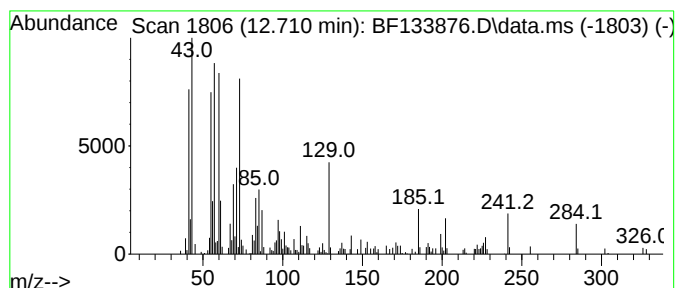
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	3.20 ng	93154	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	78
5			Isopropyl stearate	326	C21H42O2	000112-10-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

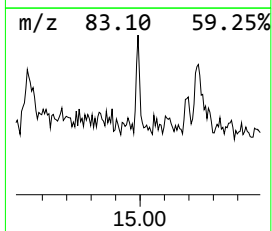
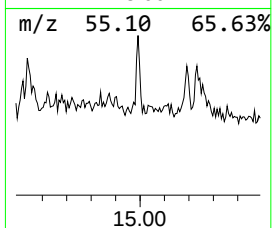
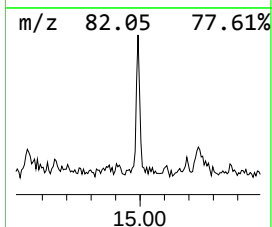
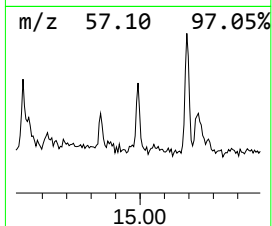
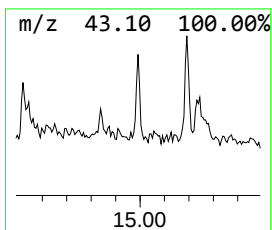
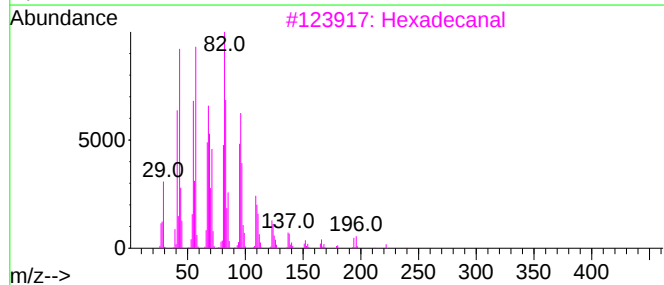
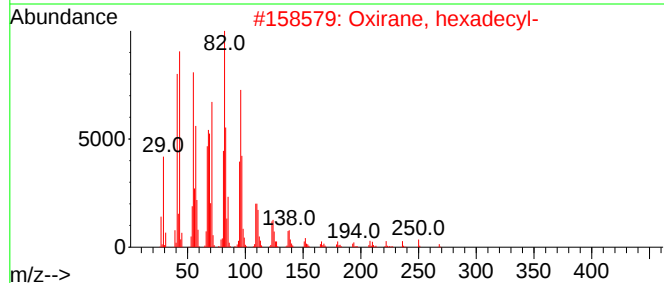
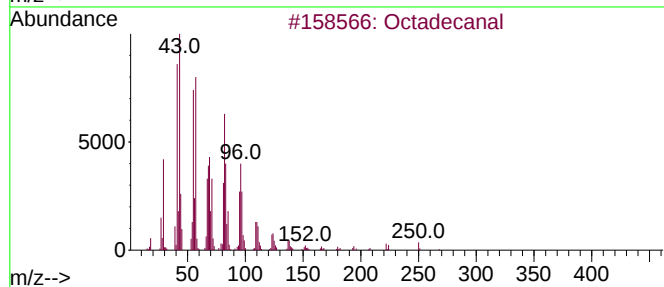
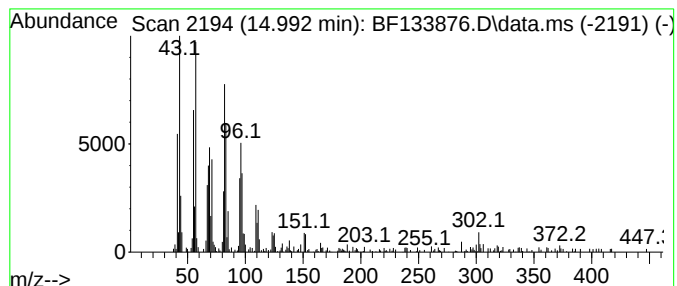
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	6.61 ng	117735	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal			268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-			268	C18H36O	007390-81-0	90
3	Hexadecanal			240	C16H32O	000629-80-1	83
4	Heptadecanal			254	C17H34O	1000376-70-0	83
5	Nonacosanal			422	C29H58O	072934-04-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

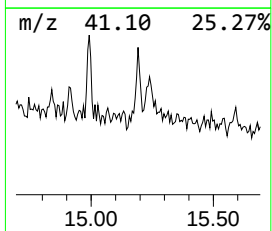
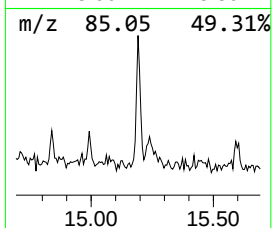
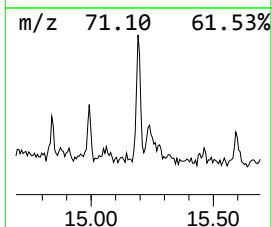
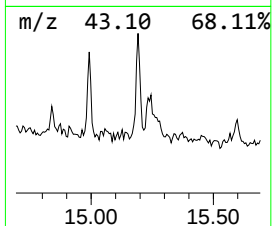
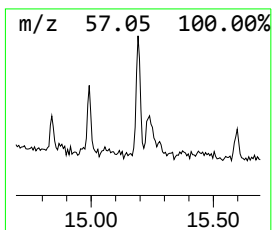
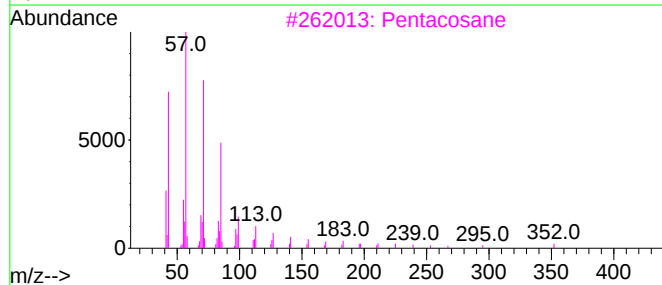
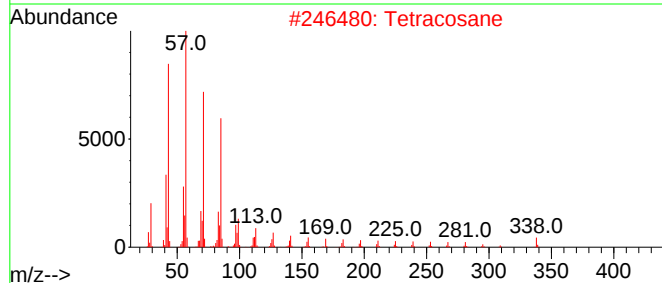
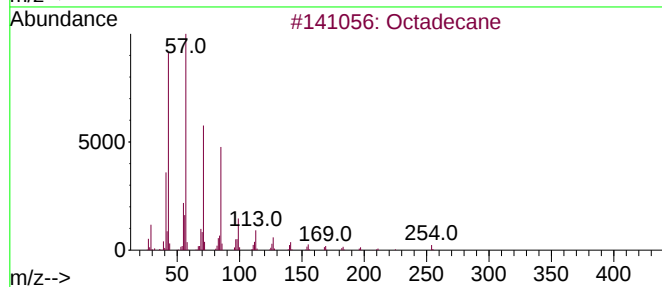
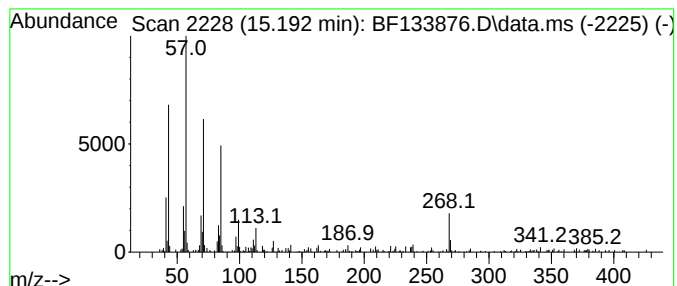
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	5.51 ng	98256	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	93
2			Tetracosane	338	C24H50	000646-31-1	91
3			Pentacosane	352	C25H52	000629-99-2	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Nonadecane	268	C19H40	000629-92-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

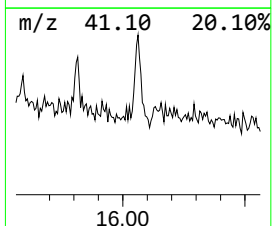
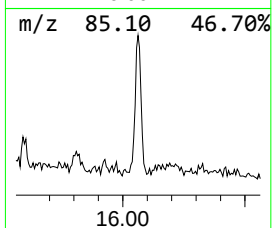
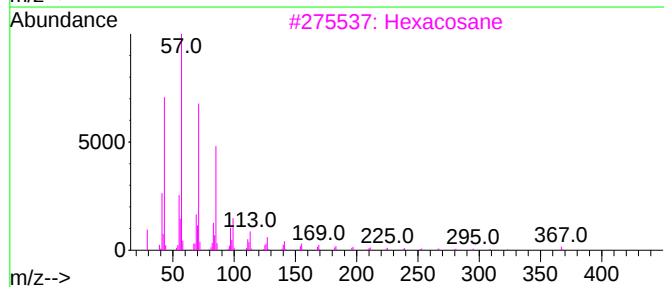
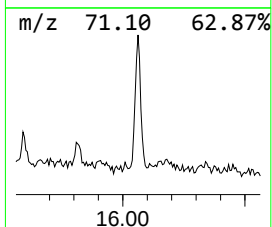
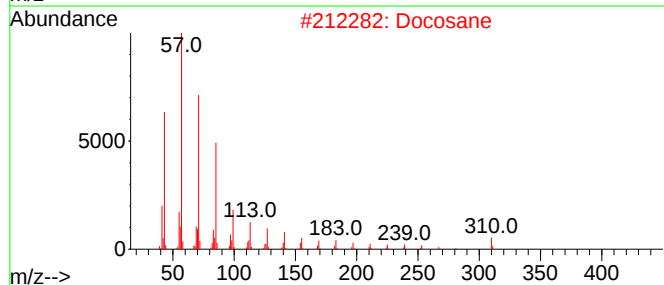
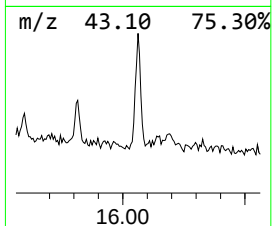
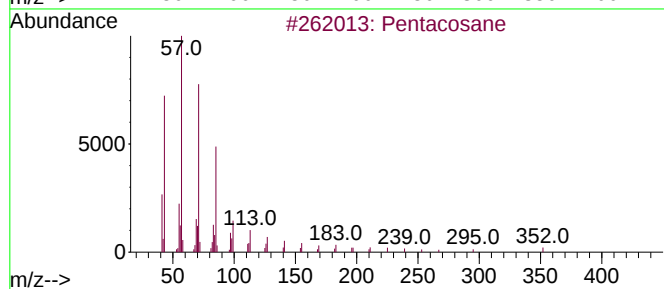
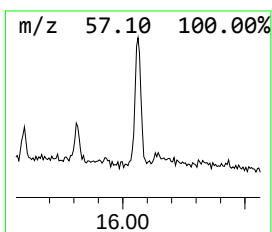
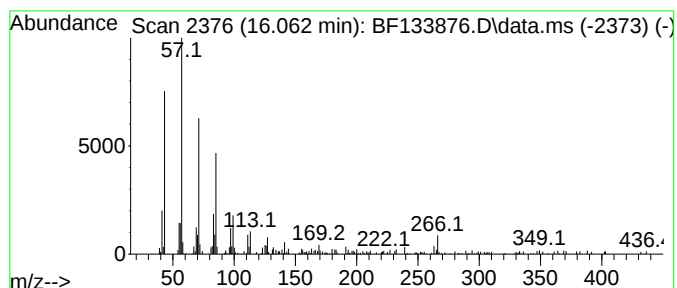
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.062	8.34 ng	148528	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	95
2			Docosane	310	C22H46	000629-97-0	93
3			Hexacosane	366	C26H54	000630-01-3	76
4			Octacosane	394	C28H58	000630-02-4	76
5			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062123\
Data File : BF133876.D
Acq On : 21 Jun 2023 17:57
Operator : CG\JU
Sample : 03296-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSIT-TW-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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
Butane, 2-metho...	2.157	21.1	ng	634633	1	6.857	602662	20.0
2-Pentanone, 4-...	5.098	32.7	ng	985063	1	6.857	602662	20.0
Benzophenone	10.610	2.9	ng	91658	3	9.898	624145	20.0
Palmitoleic acid	11.886	8.4	ng	243102	4	11.392	581714	20.0
n-Hexadecanoic ...	11.921	16.8	ng	487163	4	11.392	581714	20.0
Octadecanoic acid	12.710	3.2	ng	93154	4	11.392	581714	20.0
Octadecanal	14.992	6.6	ng	117735	6	15.557	356366	20.0
Octadecane	15.192	5.5	ng	98256	6	15.557	356366	20.0
Pentacosane	16.062	8.3	ng	148528	6	15.557	356366	20.0