

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
 Data File : BF133031.D
 Acq On : 25 Apr 2023 14:43
 Operator : CG\JU
 Sample : 02483-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S2S-TP1

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: BF133031.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.293	370	375	382	rBV	58320	75361	1.46%	0.178%
2	4.934	479	484	499	rBV	550497	827239	15.98%	1.949%
3	5.357	551	556	569	rBV	3687820	3891786	75.20%	9.168%
4	6.387	725	731	743	rBV	3585595	3945063	76.23%	9.293%
5	6.739	788	791	795	rBV	1427449	1245609	24.07%	2.934%
6	7.304	882	887	890	rBV	2812877	2528311	48.85%	5.956%
7	8.028	1006	1010	1013	rBV	2209575	1694591	32.74%	3.992%
8	9.104	1189	1193	1196	rVB	5355326	4336738	83.79%	10.216%
9	9.780	1304	1308	1311	rBV	2139764	1882775	36.38%	4.435%
10	10.492	1425	1429	1432	rBV	991485	851357	16.45%	2.005%
11	10.563	1437	1441	1455	rBV	2468438	2572911	49.71%	6.061%
12	10.804	1479	1482	1487	rBV2	39768	59412	1.15%	0.140%
13	11.257	1556	1559	1563	rBV	2291457	1960128	37.87%	4.617%
14	11.657	1624	1627	1631	rBV5	33550	67572	1.31%	0.159%
15	11.786	1643	1649	1665	rVB	1229030	2283620	44.12%	5.379%
16	11.933	1671	1674	1682	rVB2	82183	120580	2.33%	0.284%
17	12.445	1758	1761	1763	rBV2	127143	140117	2.71%	0.330%
18	12.574	1775	1783	1797	rVB	2780322	5175537	100.00%	12.192%
19	12.851	1825	1830	1833	rBV	5024642	4741169	91.61%	11.168%
20	13.563	1946	1951	1956	rBV3	35427	69770	1.35%	0.164%
21	13.757	1981	1984	1989	rVB	71175	76018	1.47%	0.179%
22	13.892	2003	2007	2011	rBV	1658733	1491959	28.83%	3.514%
23	14.074	2034	2038	2042	rVB	86655	88058	1.70%	0.207%
24	14.127	2043	2047	2054	rBV2	62517	112105	2.17%	0.264%
25	14.380	2086	2090	2095	rVB	109151	121224	2.34%	0.286%
26	14.621	2127	2131	2136	rBV2	83774	138854	2.68%	0.327%
27	14.680	2137	2141	2149	rVB	135132	176935	3.42%	0.417%
28	15.004	2192	2196	2203	rVB	136830	166772	3.22%	0.393%
29	15.139	2214	2219	2224	rBV2	72004	130327	2.52%	0.307%
30	15.315	2244	2249	2253	rBV	987823	1082649	20.92%	2.550%
31	15.368	2254	2258	2264	rVB	118396	160582	3.10%	0.378%
32	15.727	2315	2319	2323	rBV3	50536	97304	1.88%	0.229%
33	15.780	2325	2328	2335	rVB	90985	139543	2.70%	0.329%

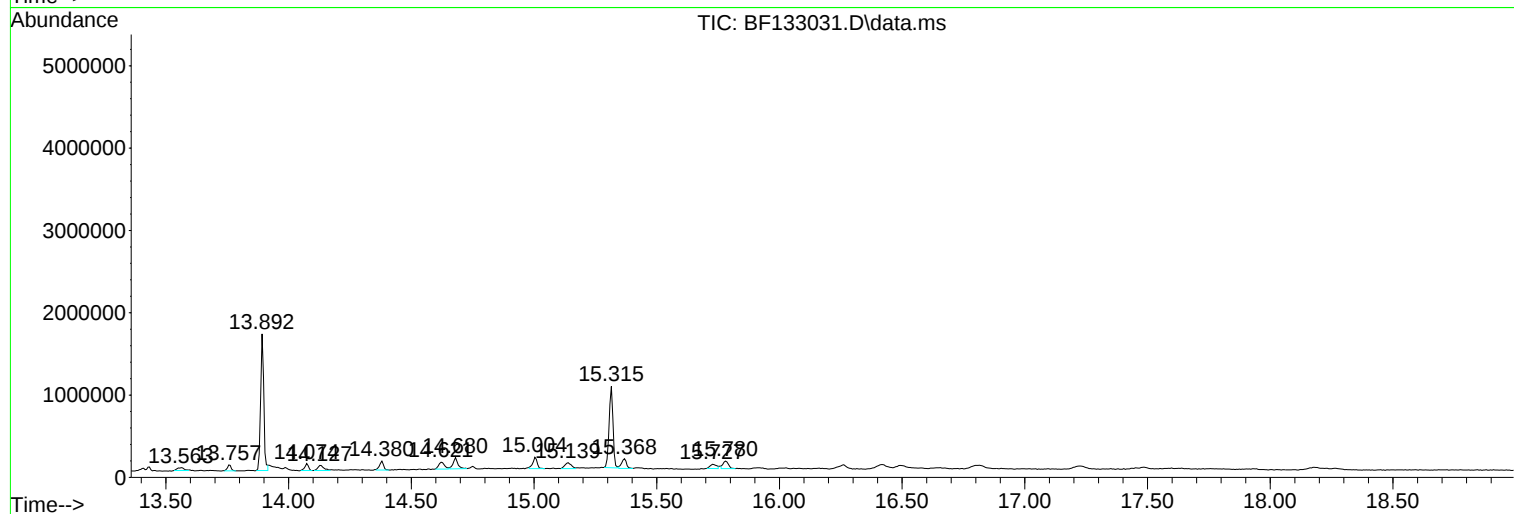
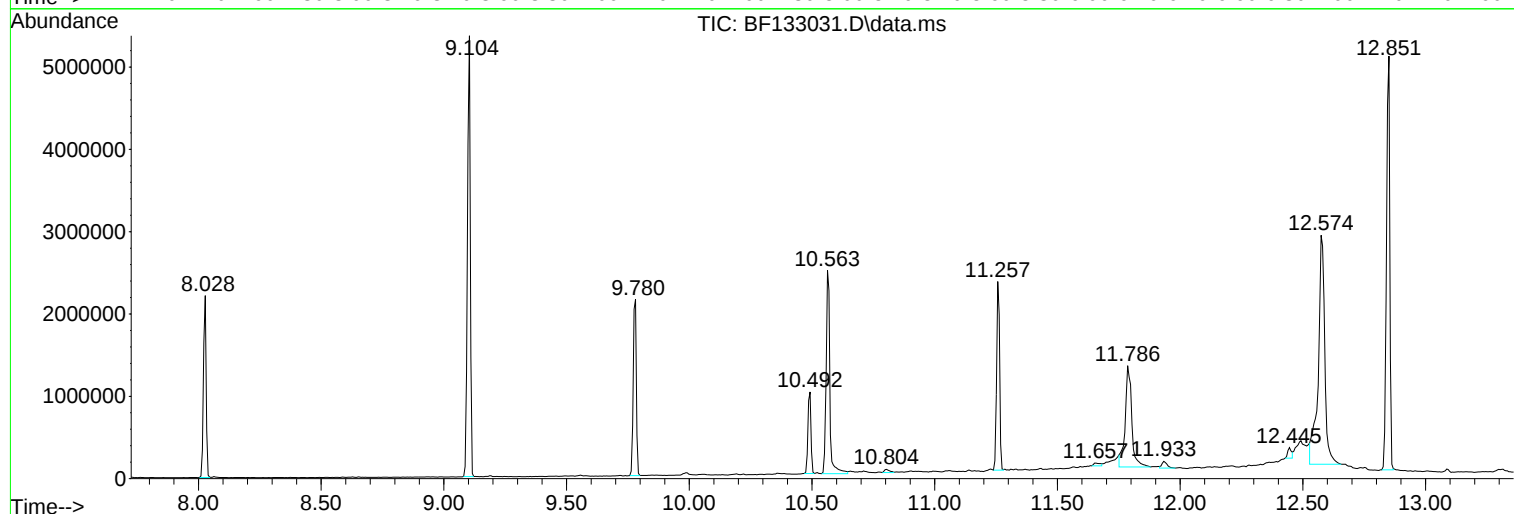
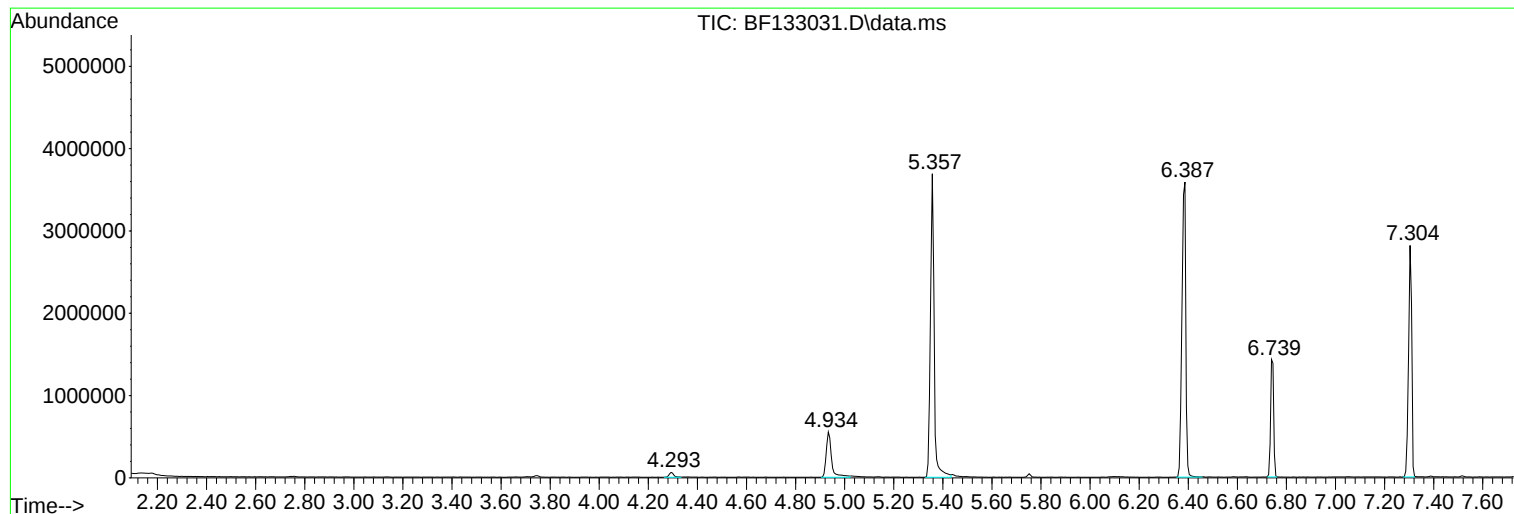
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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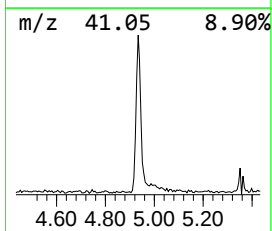
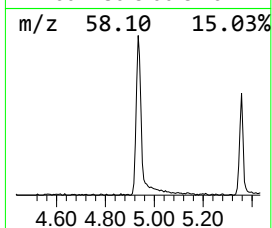
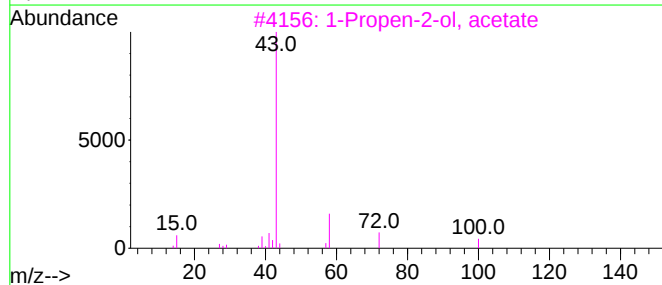
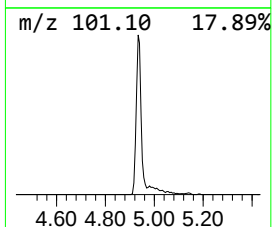
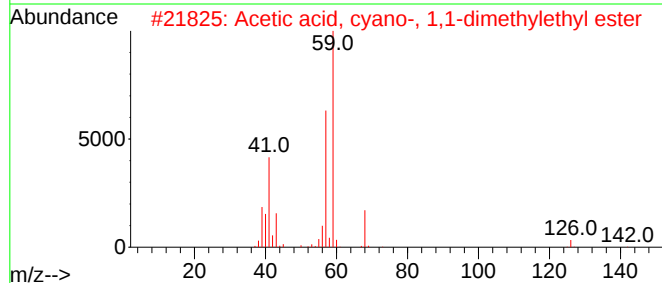
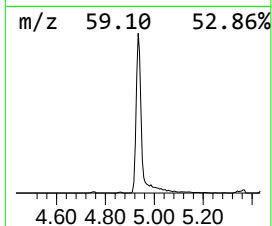
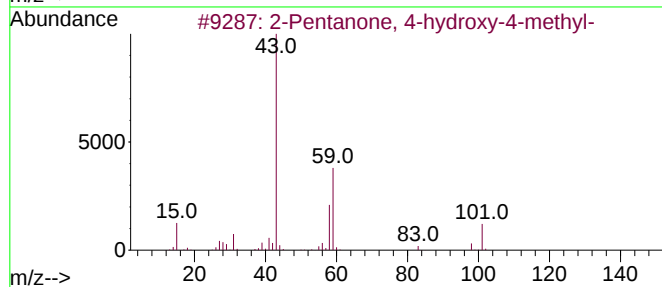
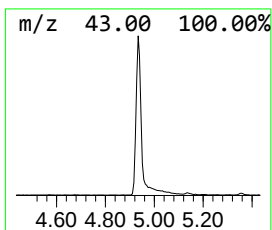
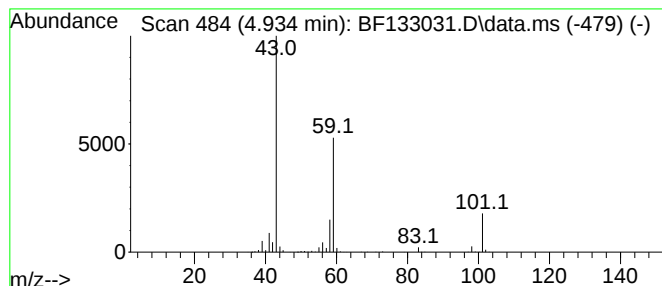
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	13.28 ng	827239	1,4-Dichlorobenzene-d4	6.745

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
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	10	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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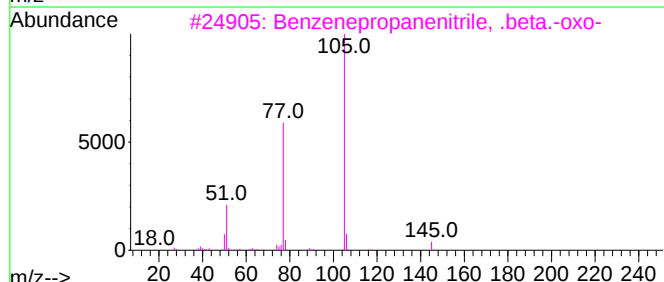
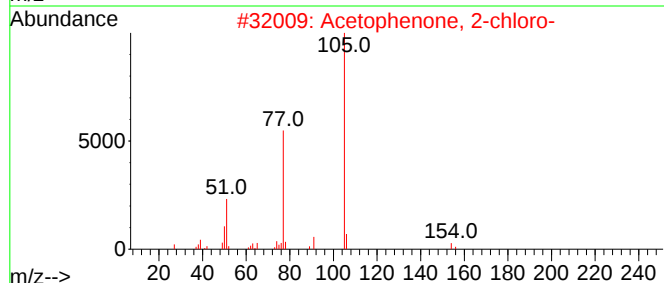
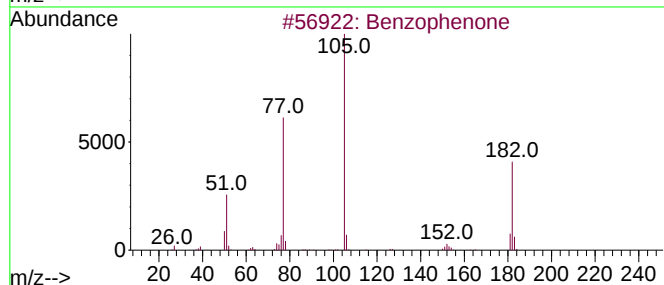
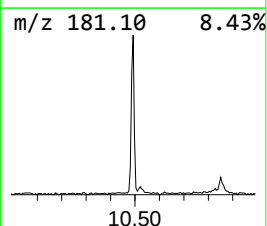
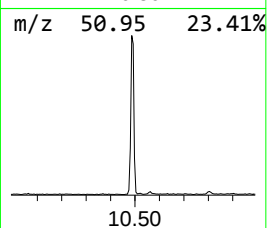
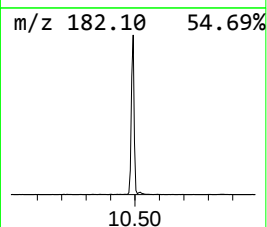
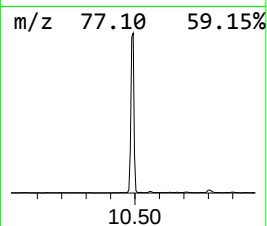
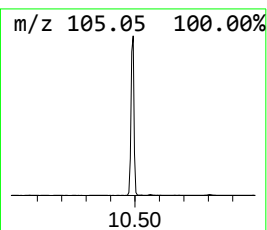
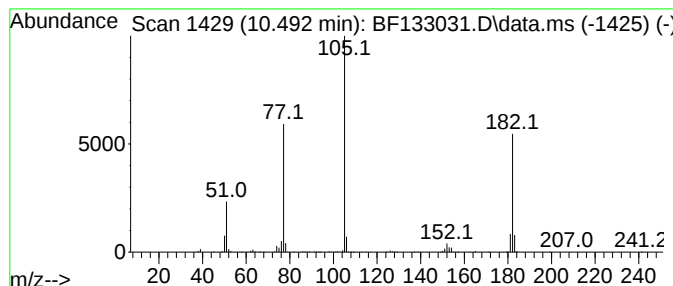
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.492	9.04 ng	851357	Acenaphthene-d10	9.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47



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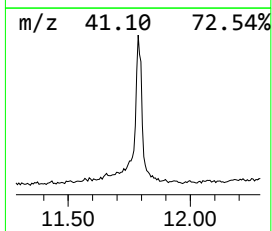
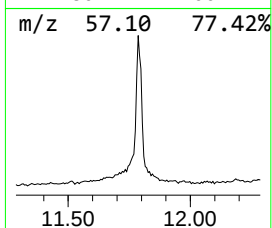
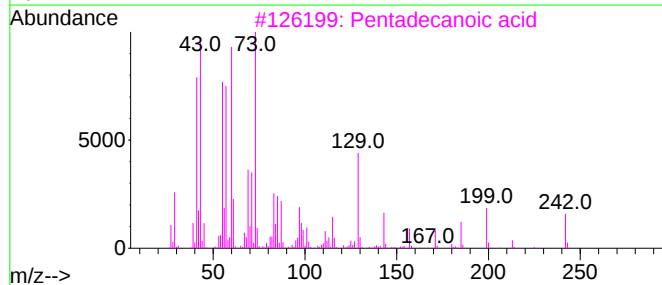
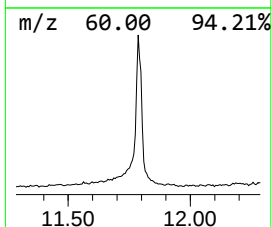
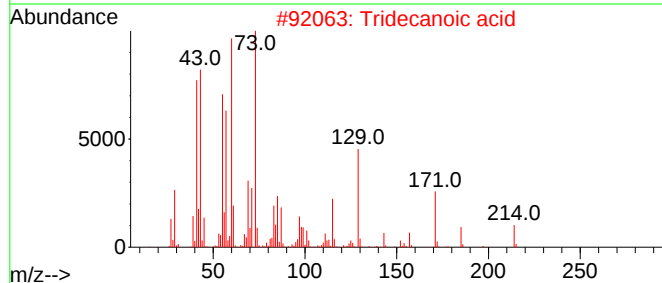
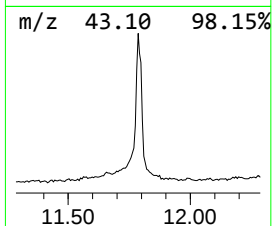
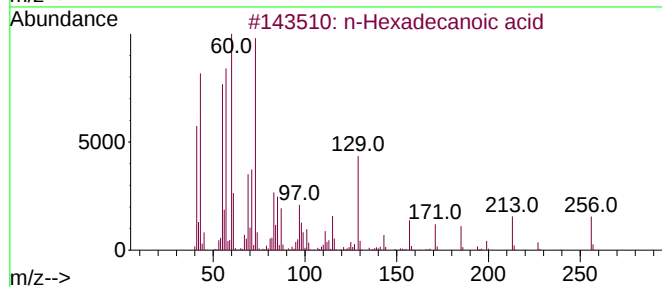
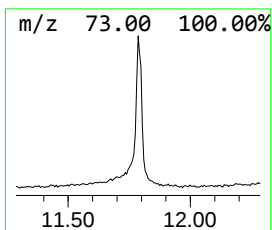
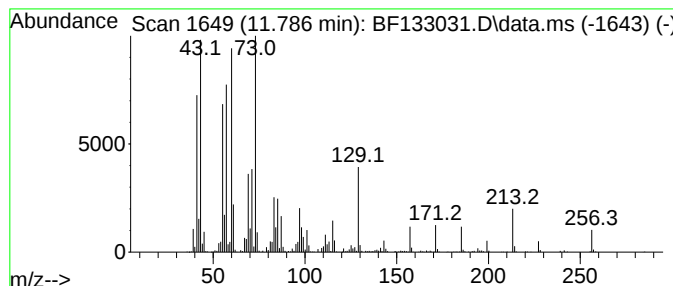
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	23.30 ng	2283620	Phenanthrene-d10	11.257

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	89
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	70



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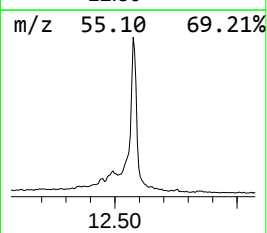
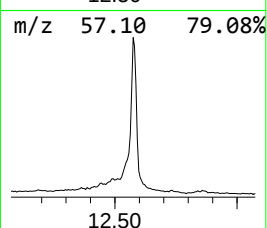
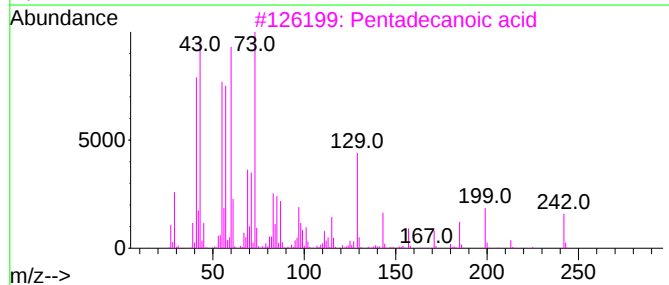
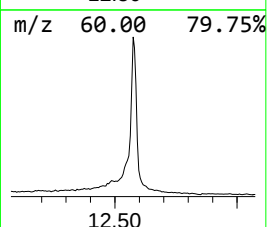
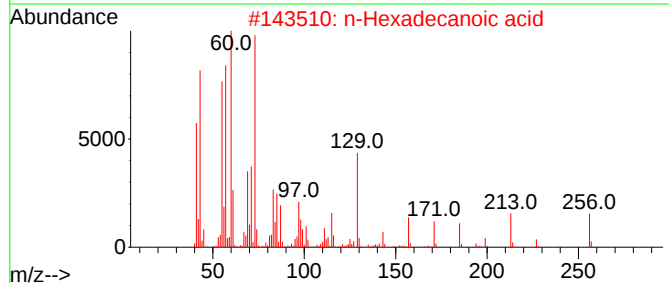
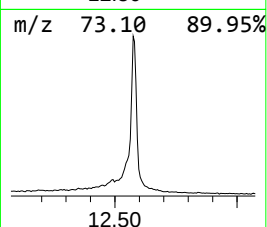
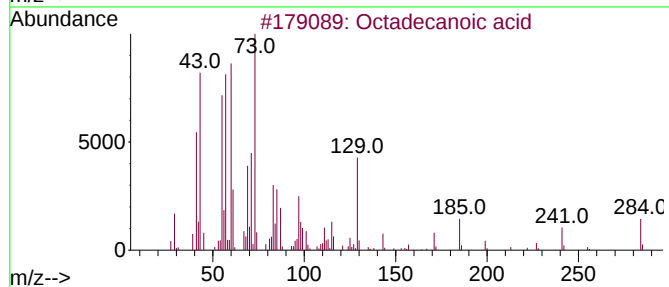
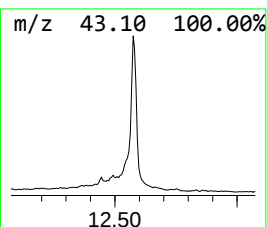
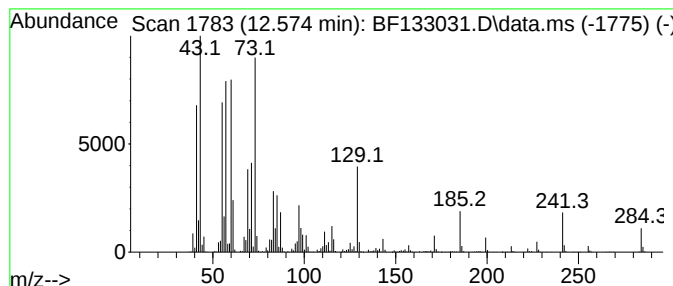
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	69.38 ng	5175540	Chrysene-d12	13.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80



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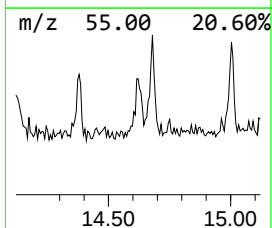
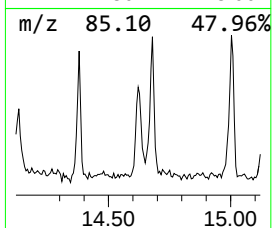
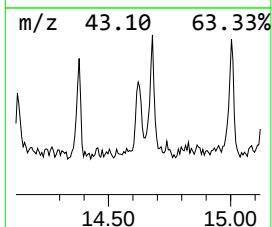
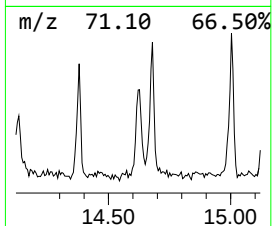
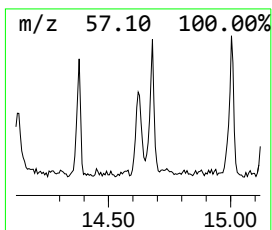
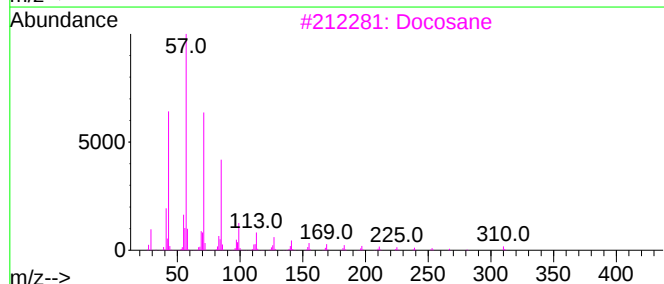
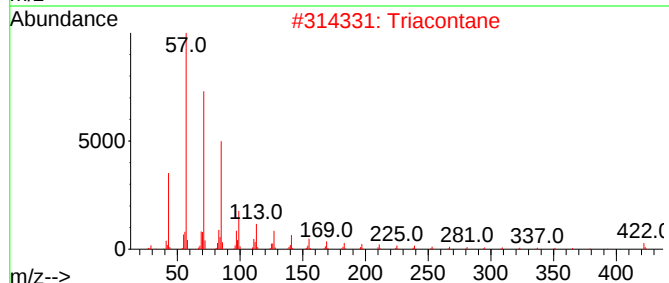
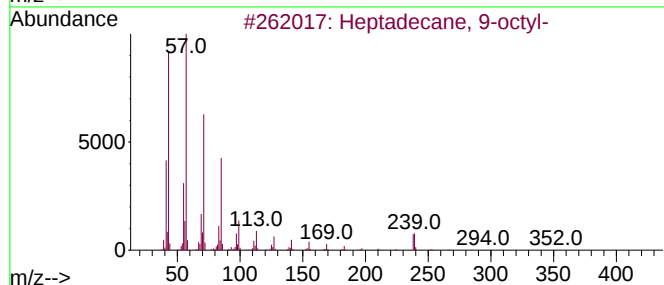
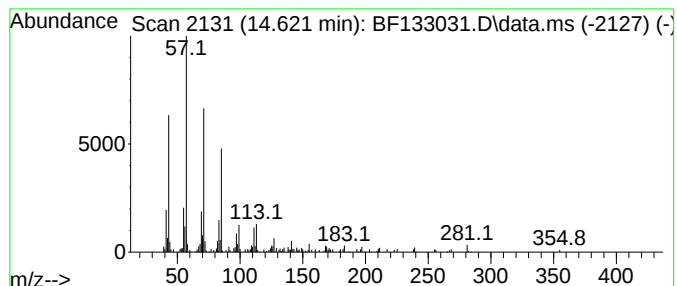
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Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.621	2.57 ng	138854	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2			Triacontane	422	C30H62	000638-68-6	87
3			Docosane	310	C22H46	000629-97-0	87
4			Heptacosane	380	C27H56	000593-49-7	87
5			Octadecane	254	C18H38	000593-45-3	83



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ALS Vial : 10 Sample Multiplier: 1

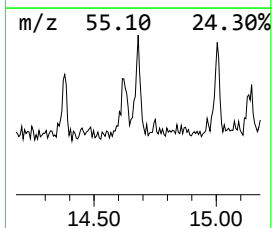
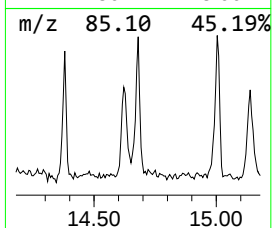
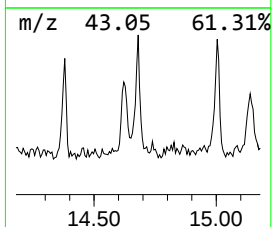
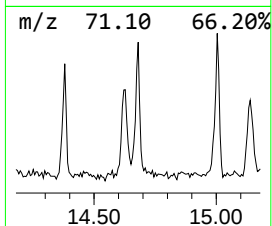
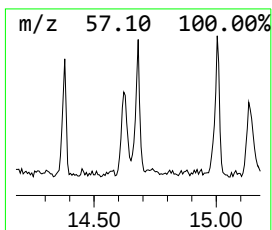
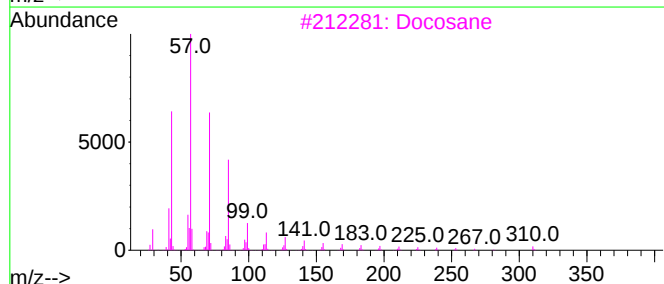
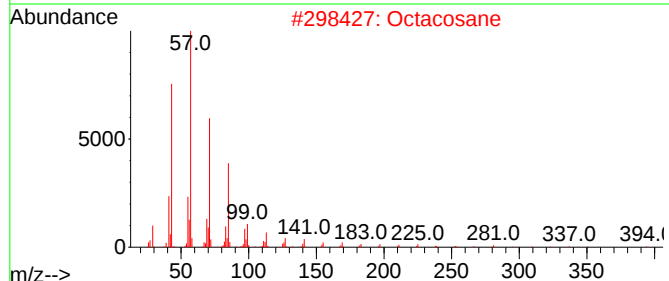
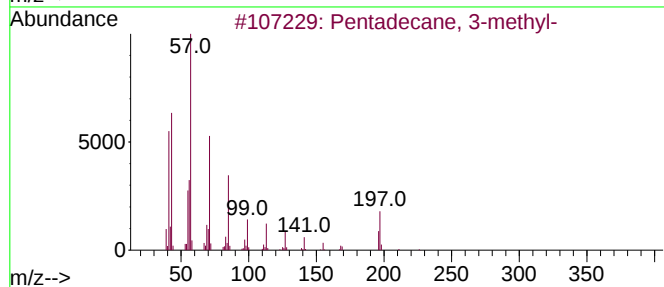
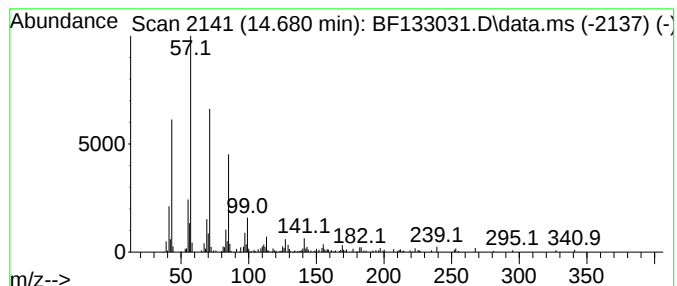
Instrument :
BNA_F
ClientSampleId :
S2S-TP1

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

Peak Number 6 Pentadecane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.680	3.27 ng	176935	Perylene-d12	15.315	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 3-methyl-	226	C16H34	002882-96-4	87
2	Octacosane	394	C28H58	000630-02-4	83
3	Docosane	310	C22H46	000629-97-0	83
4	Octadecane	254	C18H38	000593-45-3	83
5	Hexacosane	366	C26H54	000630-01-3	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133031.D
Acq On : 25 Apr 2023 14:43
Operator : CG\JU
Sample : 02483-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

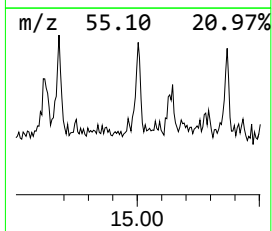
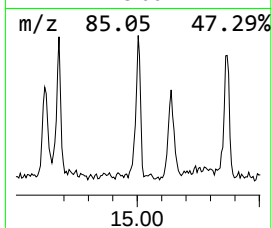
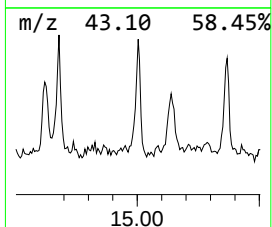
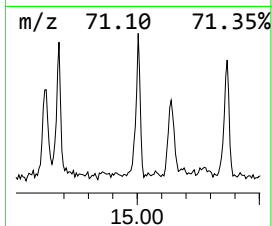
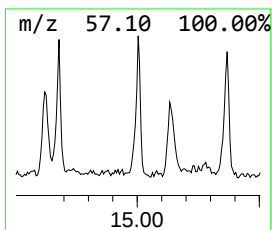
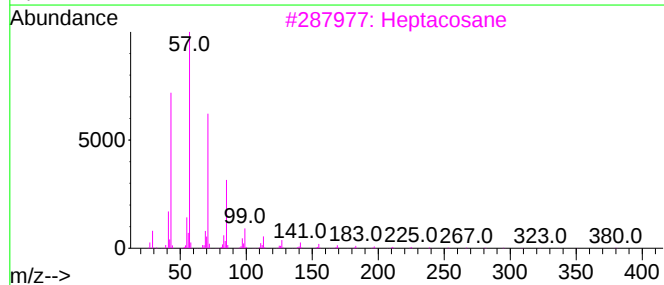
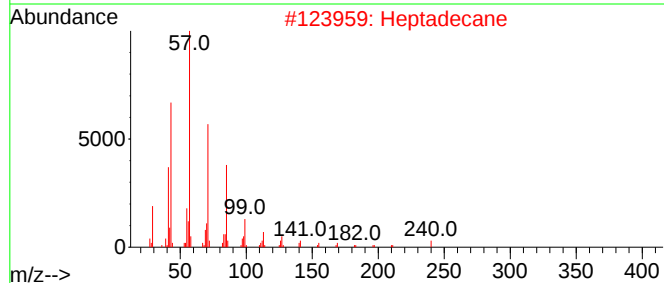
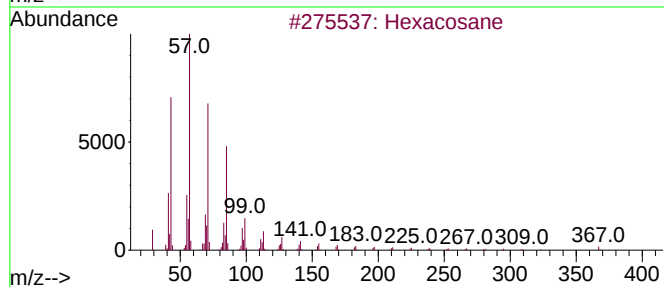
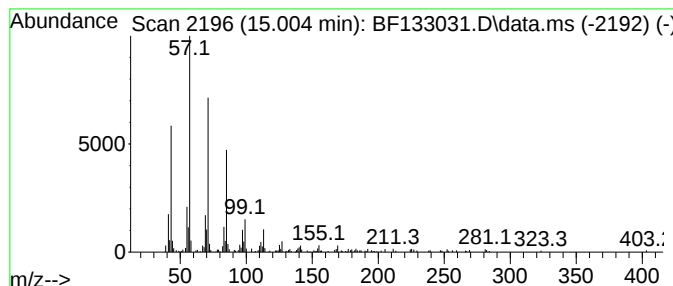
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.004	3.08 ng	166772	Perylene-d12	15.315	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heptadecane	240	C17H36	000629-78-7	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133031.D
Acq On : 25 Apr 2023 14:43
Operator : CG\JU
Sample : 02483-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2S-TP1

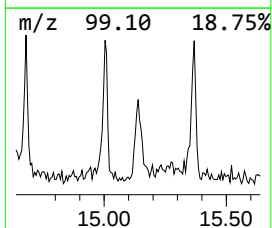
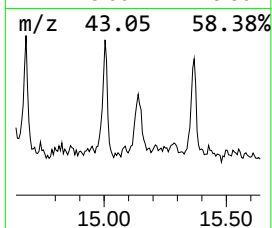
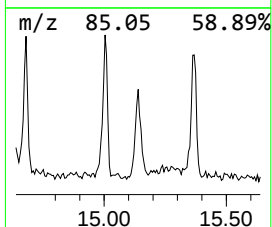
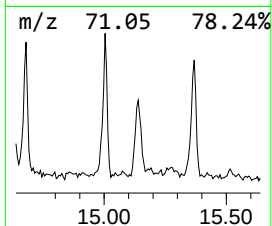
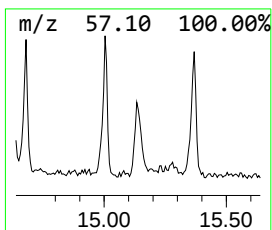
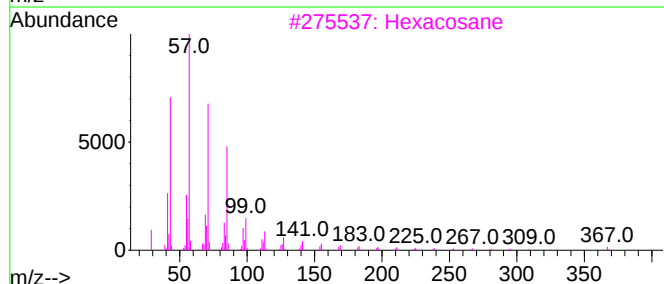
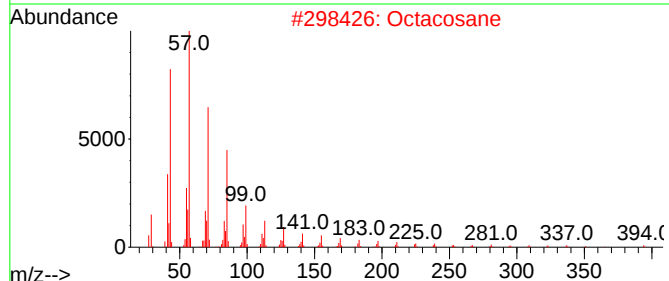
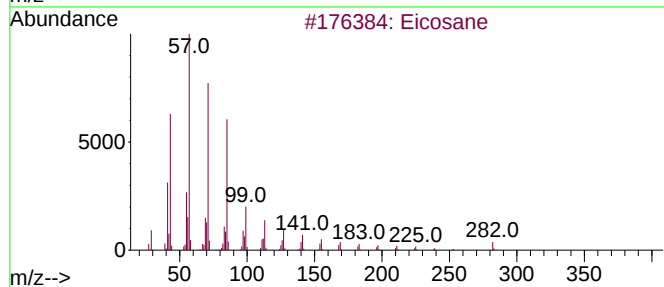
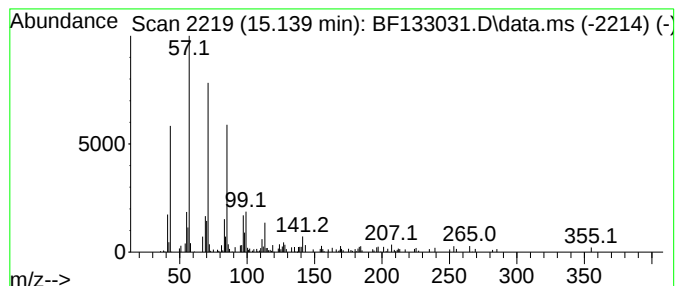
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	2.41 ng	130327	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
5			Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133031.D
Acq On : 25 Apr 2023 14:43
Operator : CG\JU
Sample : 02483-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S2S-TP1

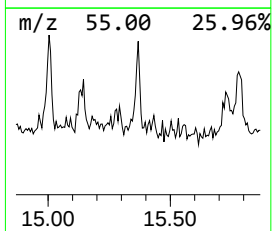
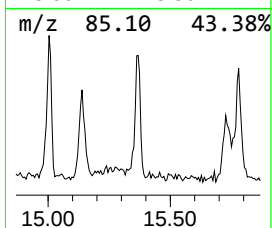
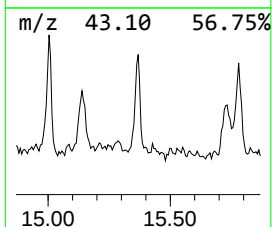
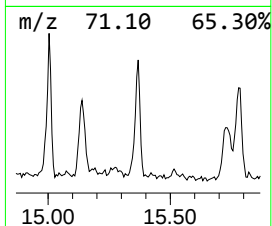
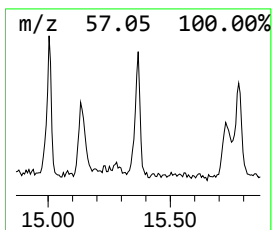
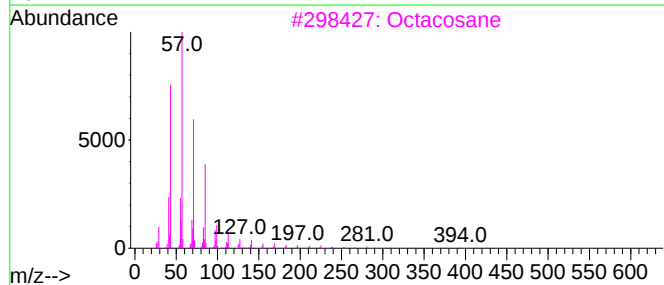
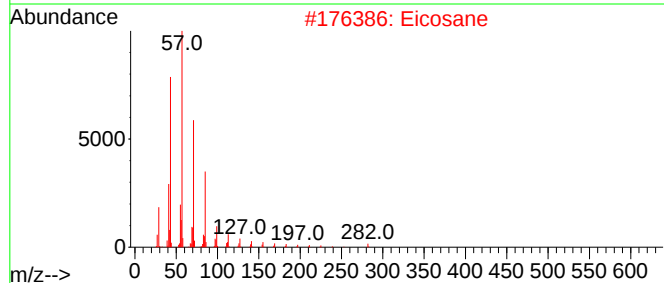
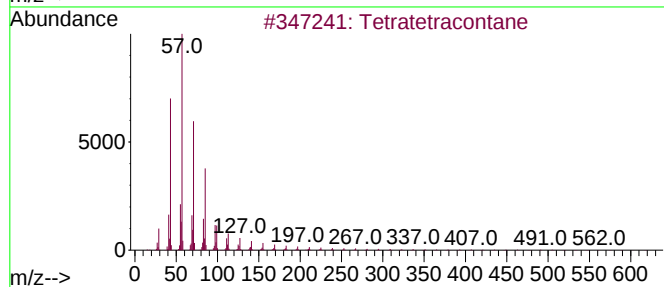
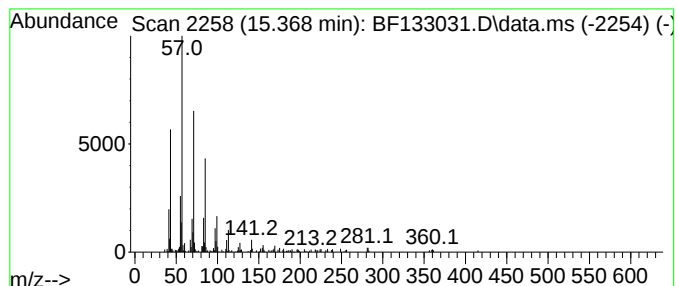
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	2.97 ng	160582	Perylene-d12	15.315

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	90
2			Eicosane	282	C20H42	000112-95-8	90
3			Octacosane	394	C28H58	000630-02-4	90
4			Hexacosane	366	C26H54	000630-01-3	87
5			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133031.D
Acq On : 25 Apr 2023 14:43
Operator : CG\JU
Sample : 02483-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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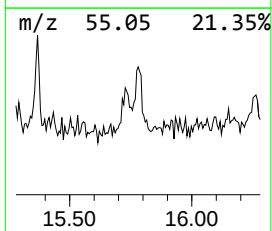
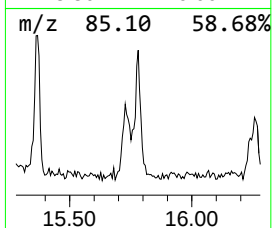
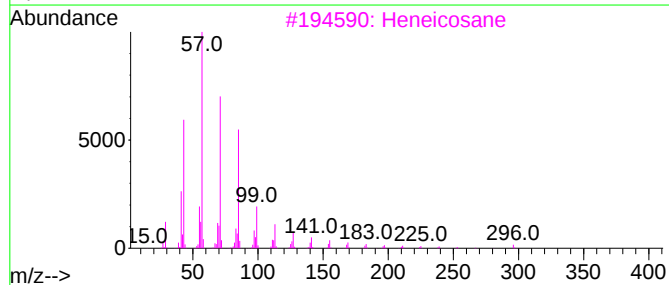
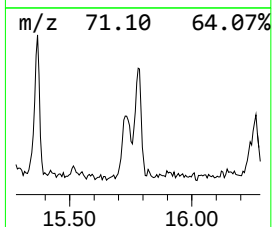
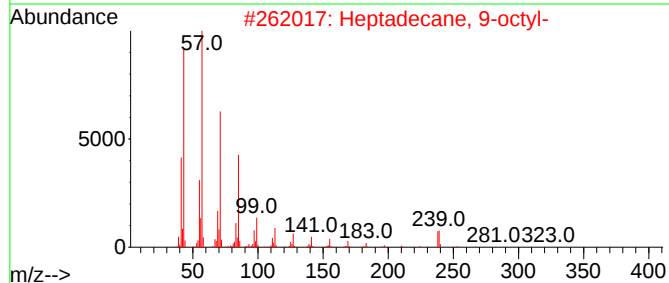
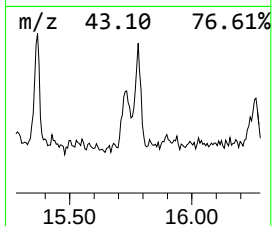
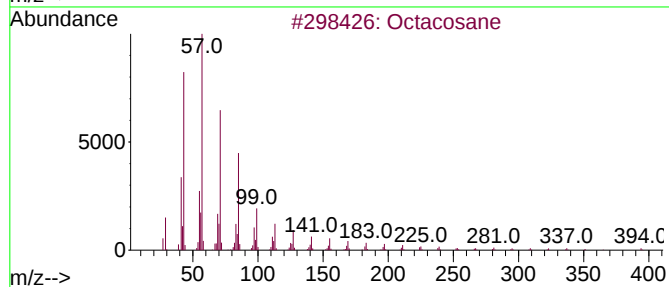
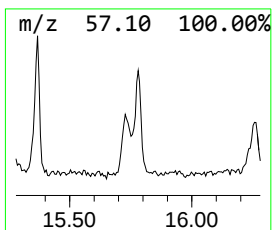
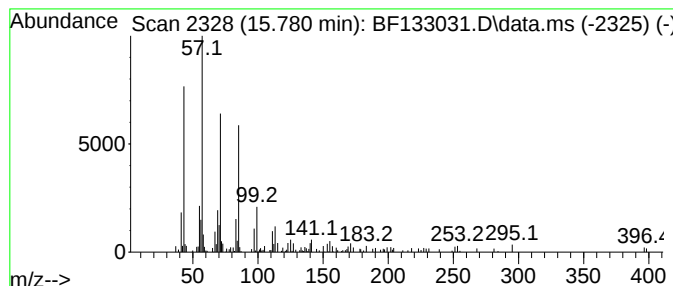
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.780	2.58 ng	139543	Perylene-d12	15.315

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	87
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3		Heneicosane	296	C21H44	000629-94-7	86
4		Tetracosane	338	C24H50	000646-31-1	86
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042523\
Data File : BF133031.D
Acq On : 25 Apr 2023 14:43
Operator : CG\JU
Sample : 02483-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzophenone	10.492	9.0	ng	851357	3	9.780	1882780	20.0
n-Hexadecanoic ...	11.786	23.3	ng	2283620	4	11.257	1960130	20.0
Octadecanoic acid	12.574	69.4	ng	5175540	5	13.892	1491960	20.0
Heptadecane, 9-...	14.621	2.6	ng	138854	6	15.315	1082650	20.0
Pentadecane, 3-...	14.680	3.3	ng	176935	6	15.315	1082650	20.0
Hexacosane	15.004	3.1	ng	166772	6	15.315	1082650	20.0
Eicosane	15.139	2.4	ng	130327	6	15.315	1082650	20.0
Tetratetracontane	15.368	3.0	ng	160582	6	15.315	1082650	20.0
Octacosane	15.780	2.6	ng	139543	6	15.315	1082650	20.0