

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030425\
 Data File : BF141827.D
 Acq On : 04 Mar 2025 15:19
 Operator : RC/JU
 Sample : Q1480-25
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF022725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	13	23	31	rVB	1959698	3235833	35.27%	4.729%
2	5.510	574	581	586	rBV	5440991	7696416	83.90%	11.247%
3	6.504	743	750	756	rBV	5247100	7801772	85.05%	11.401%
4	6.887	809	815	820	rVB	1252172	1566423	17.08%	2.289%
5	7.445	903	910	915	rBV	3627434	5175706	56.42%	7.563%
6	7.692	948	952	961	rVB	125983	157909	1.72%	0.231%
7	8.163	1026	1032	1037	rBV	1628898	2108302	22.98%	3.081%
8	9.239	1208	1215	1220	rBV	6623719	9173356	100.00%	13.405%
9	9.916	1321	1330	1335	rBV	1876177	2358482	25.71%	3.446%
10	10.322	1393	1399	1411	rVB	49587	94792	1.03%	0.139%
11	10.628	1444	1451	1457	rBV	684147	900924	9.82%	1.317%
12	10.704	1457	1464	1469	rBV	4276418	5611936	61.18%	8.201%
13	11.404	1577	1583	1589	rVB	1727310	2243970	24.46%	3.279%
14	11.633	1616	1622	1629	rBV	109900	181823	1.98%	0.266%
15	11.927	1662	1672	1694	rBV2	1631781	3085263	33.63%	4.509%
16	12.180	1710	1715	1724	rVB	199069	260540	2.84%	0.381%
17	12.627	1785	1791	1797	rBV3	83472	197429	2.15%	0.289%
18	12.710	1798	1805	1818	rVV	967827	1694069	18.47%	2.476%
19	12.986	1846	1852	1858	rBV	5925370	7866019	85.75%	11.495%
20	13.286	1898	1903	1910	rVB	84250	158582	1.73%	0.232%
21	13.569	1945	1951	1958	rVB	1214434	1953259	21.29%	2.854%
22	13.880	1998	2004	2016	rBV	410056	777014	8.47%	1.135%
23	14.033	2024	2030	2039	rVB	1224289	1684156	18.36%	2.461%
24	14.363	2081	2086	2091	rVB	93122	143873	1.57%	0.210%
25	14.516	2107	2112	2124	rBV2	84713	184193	2.01%	0.269%
26	14.663	2133	2137	2145	rVB	102143	158161	1.72%	0.231%
27	14.816	2158	2163	2169	rBV	116173	193574	2.11%	0.283%
28	15.310	2243	2247	2252	rVB	62038	99999	1.09%	0.146%
29	15.510	2275	2281	2286	rBV	892148	1387362	15.12%	2.027%
30	16.921	2516	2521	2535	rVB4	99605	280286	3.06%	0.410%

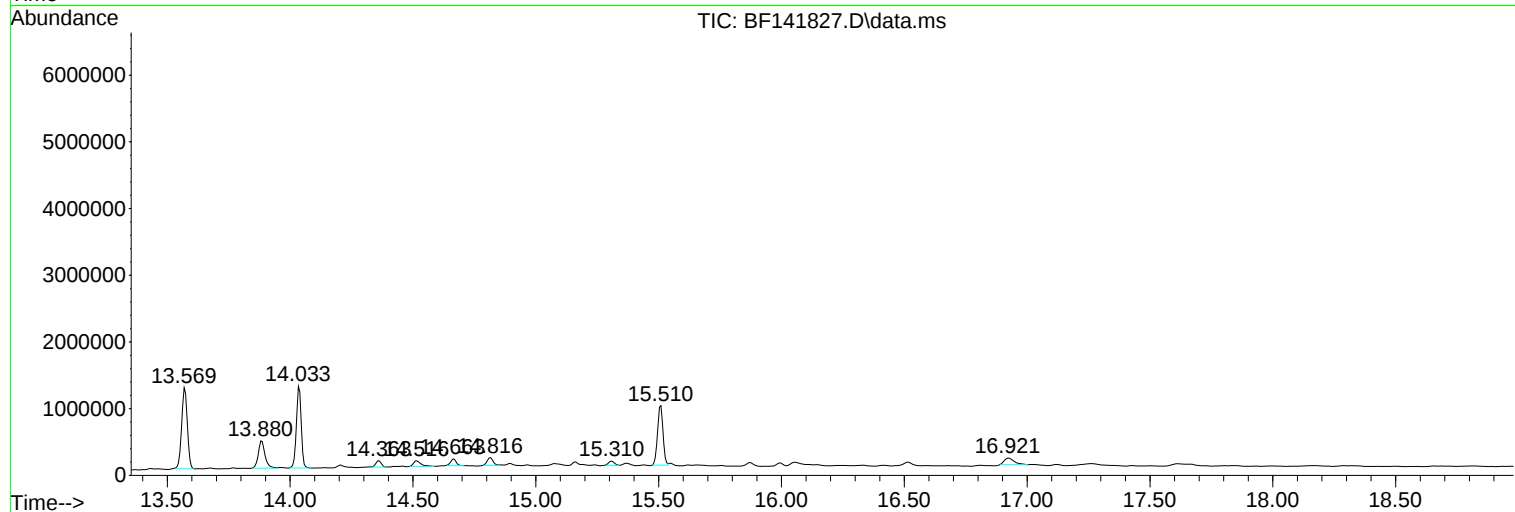
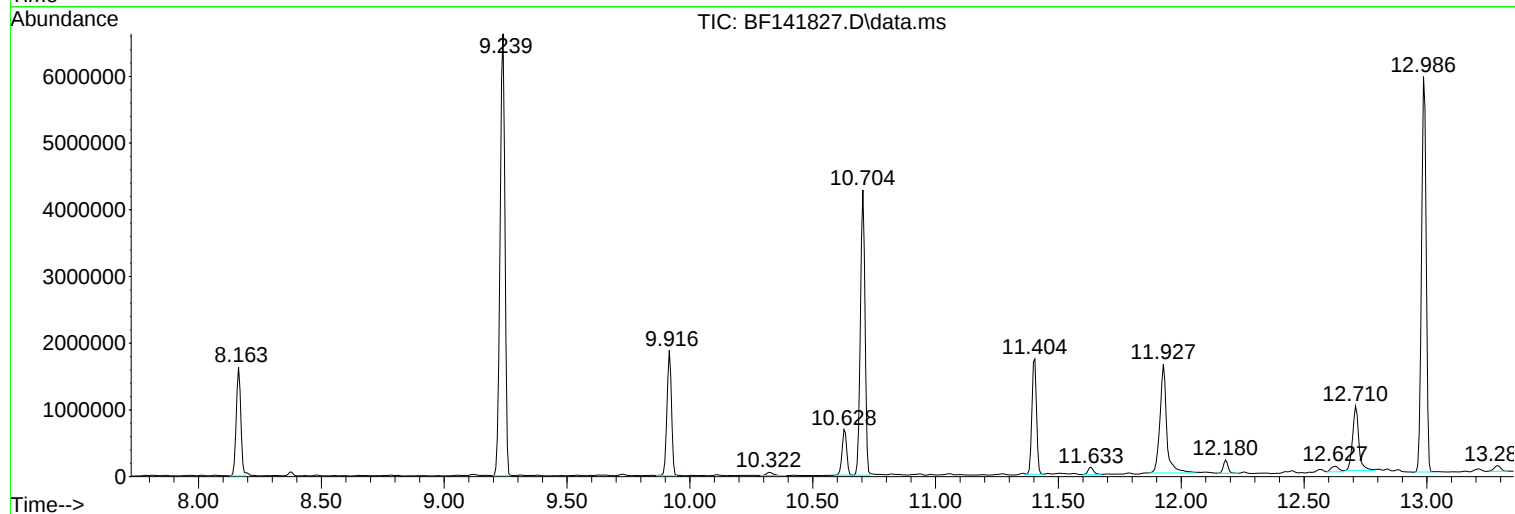
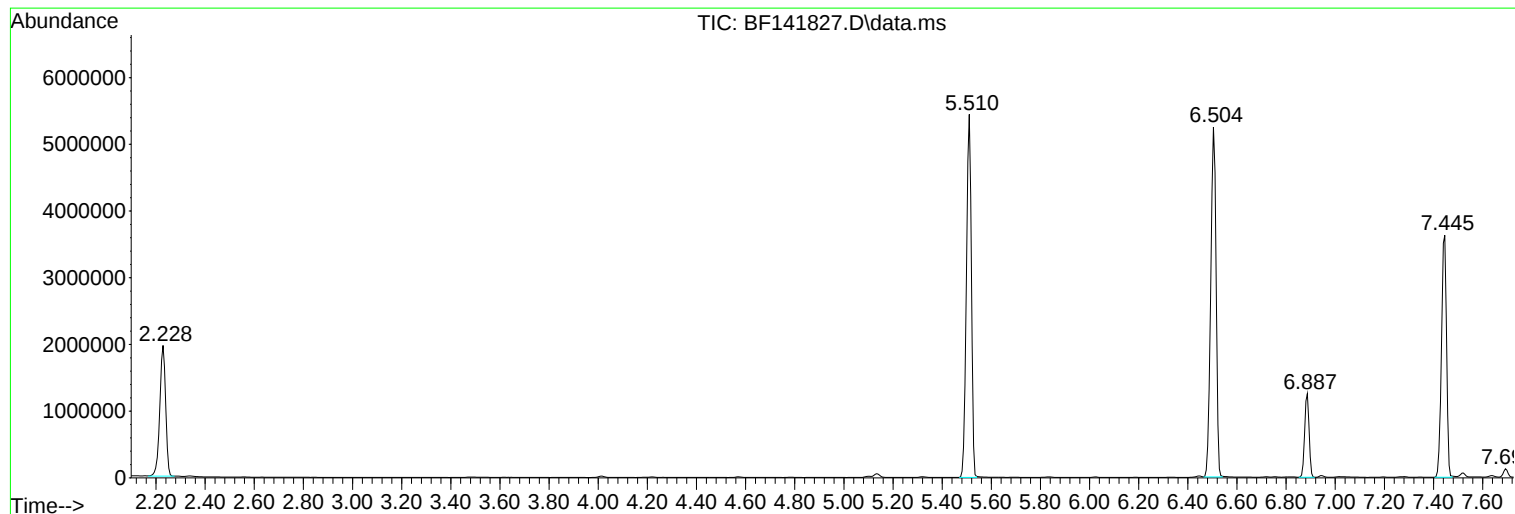
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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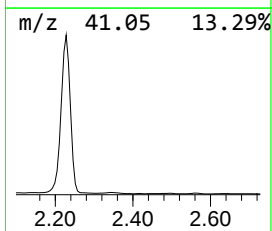
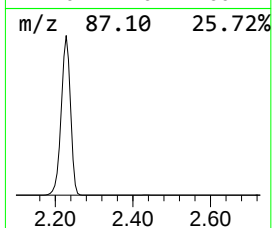
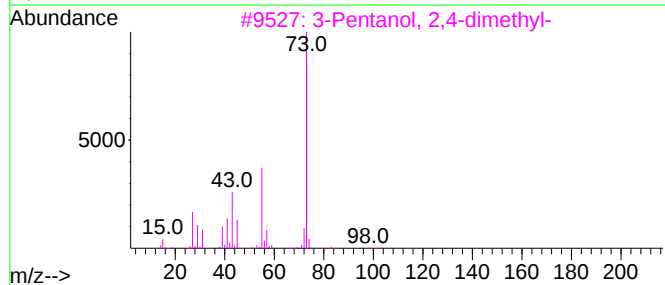
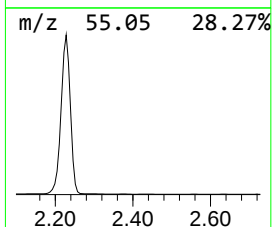
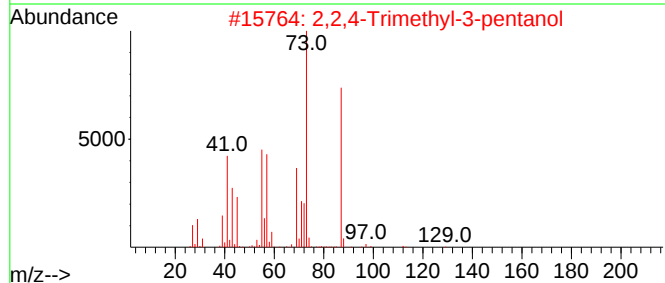
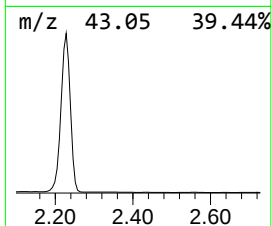
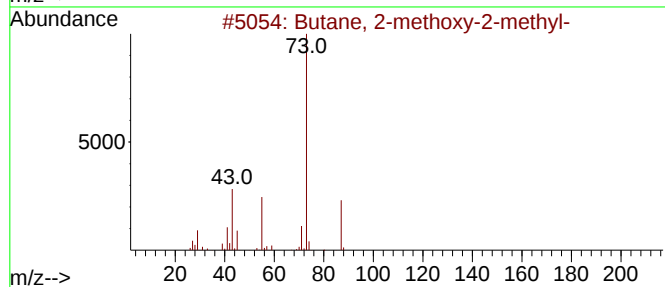
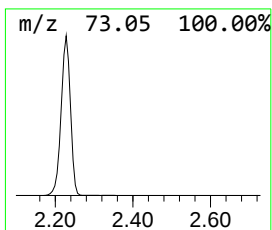
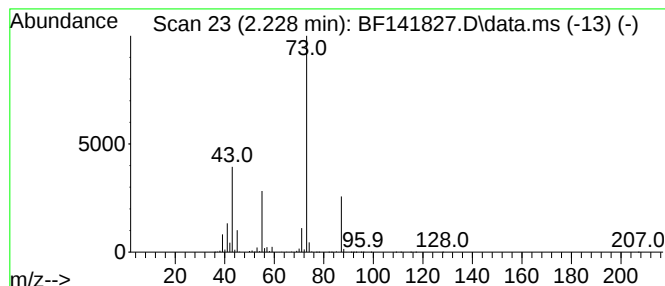
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	41.31 ng	3235830	1,4-Dichlorobenzene-d4	6.887

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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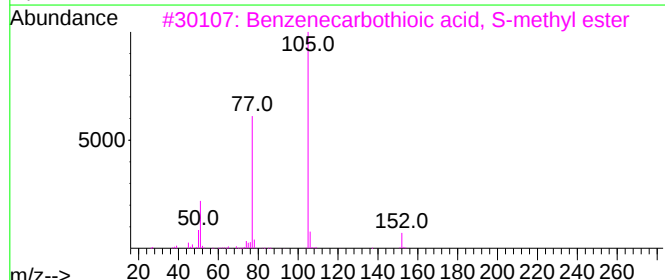
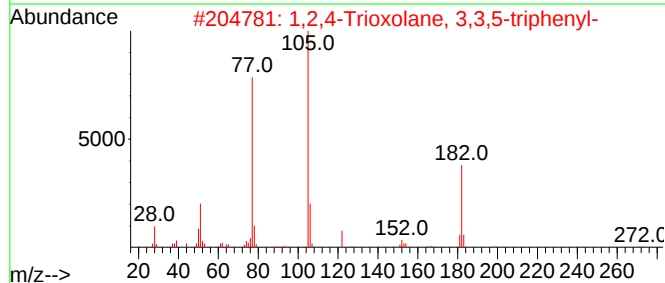
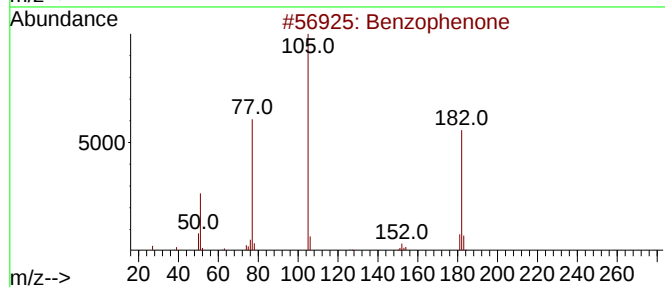
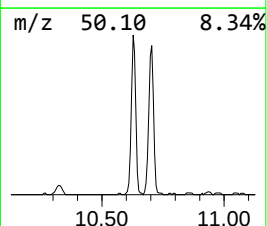
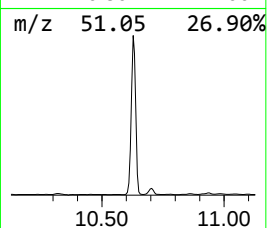
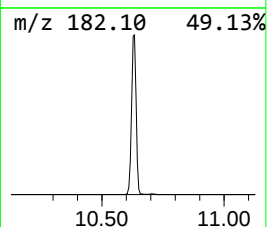
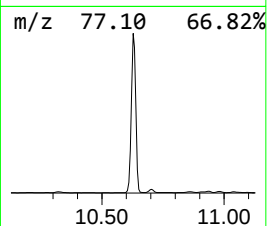
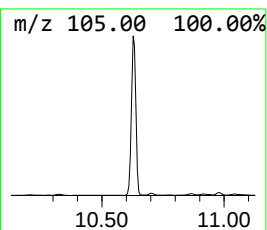
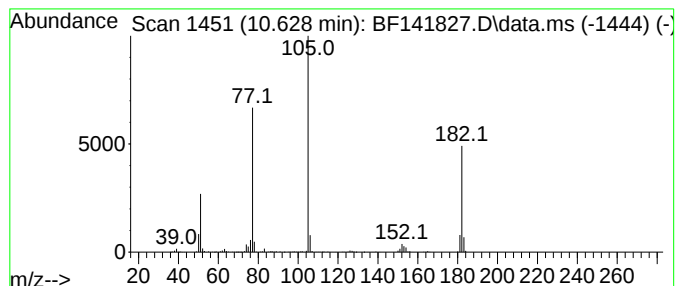
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	7.64 ng	900924	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	72
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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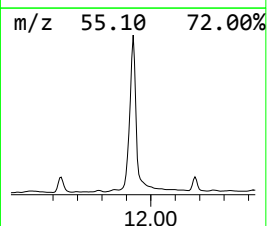
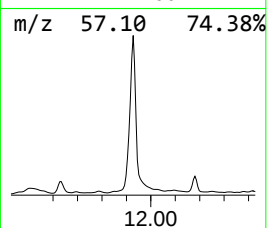
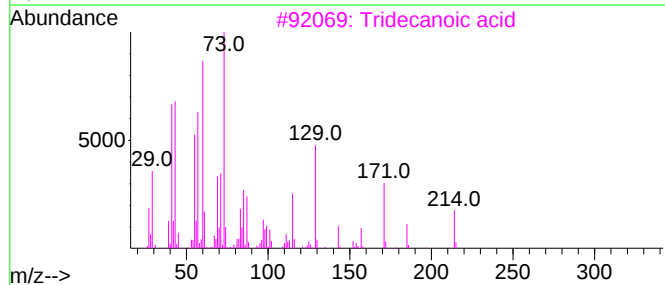
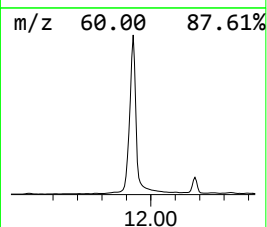
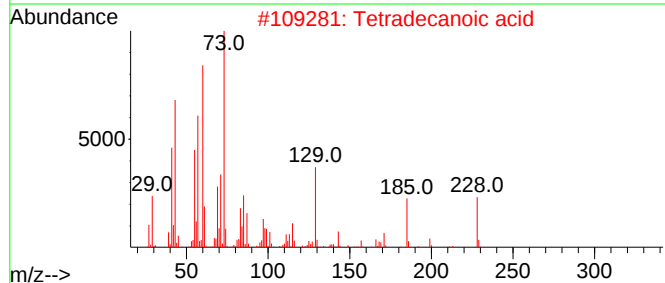
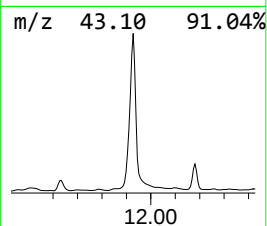
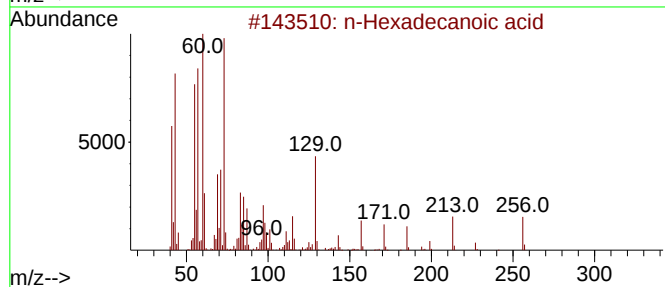
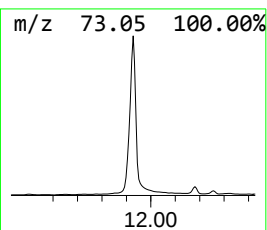
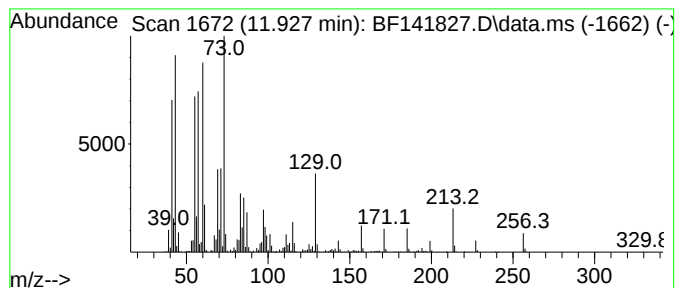
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	27.50 ng	3085260	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	55



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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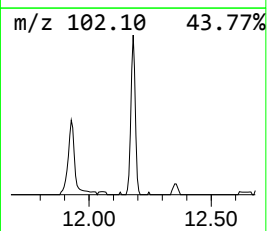
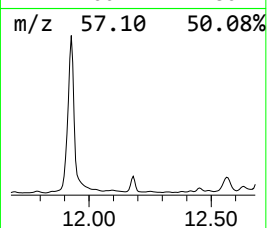
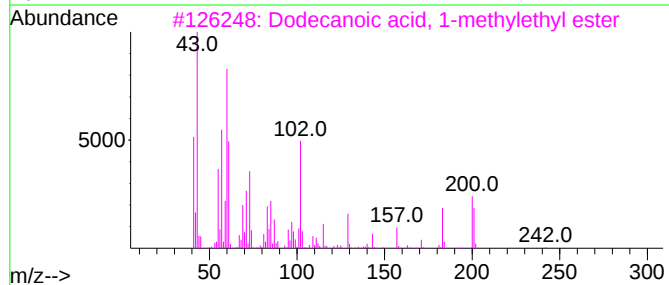
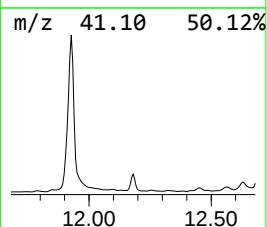
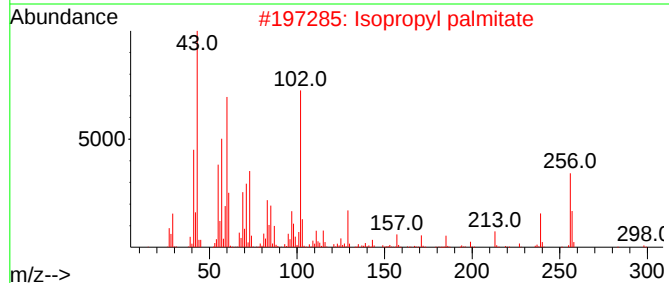
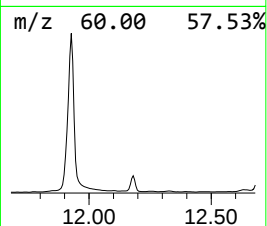
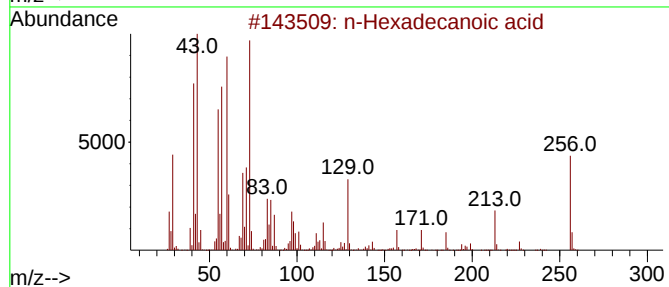
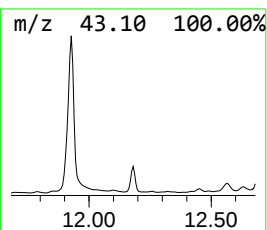
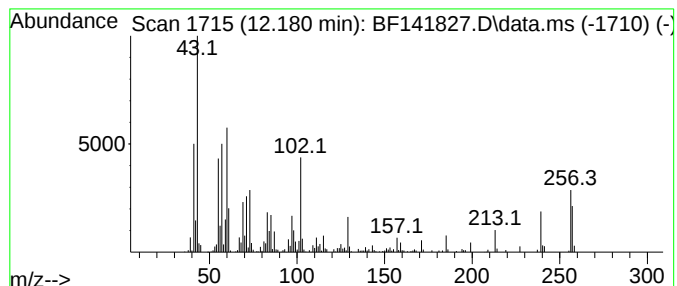
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Isopropyl palmitate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.180	2.32 ng	260540	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Isopropyl palmitate	298	C19H38O2	000142-91-6	62
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	46
4			i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	42
5			8-Methylnonanoic acid, isopropyl...	214	C13H26O2	1000452-00-6	38



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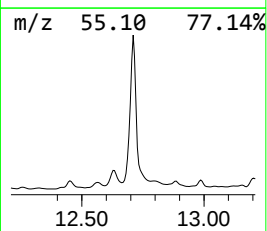
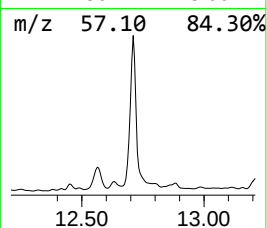
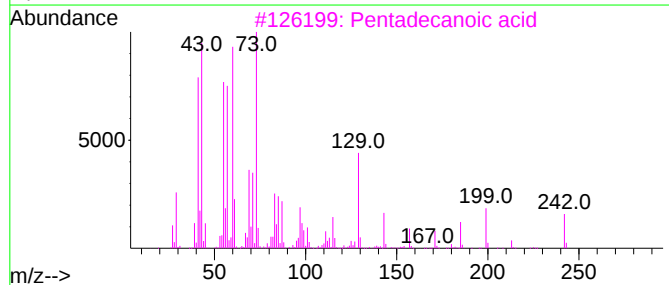
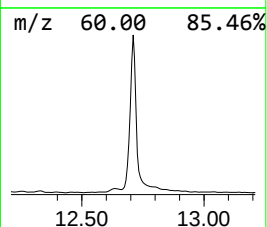
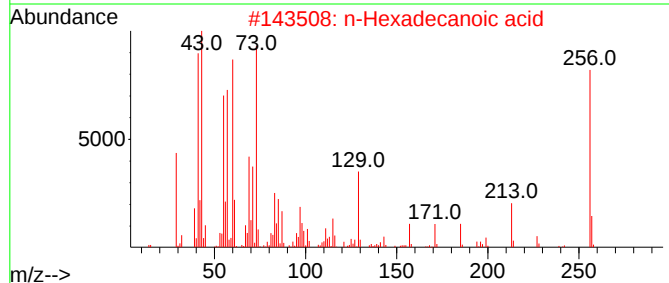
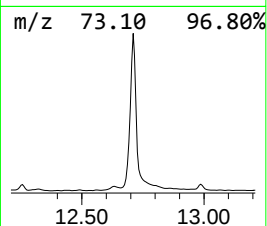
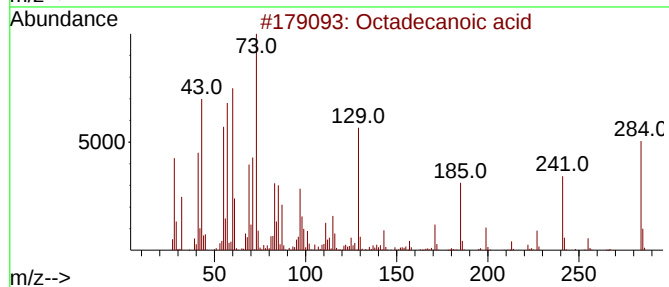
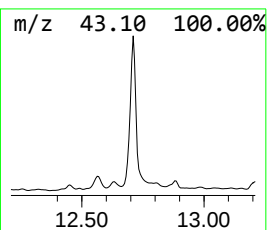
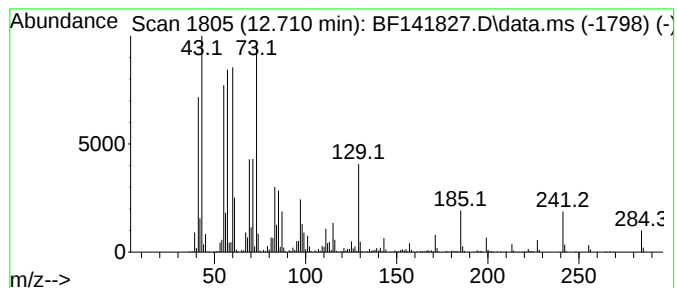
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	15.10 ng	1694070	Phenanthrene-d10	11.404

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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Misc :
ALS Vial : 5 Sample Multiplier: 1

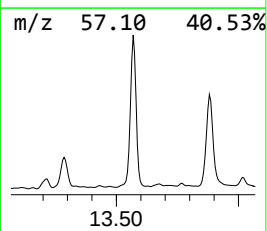
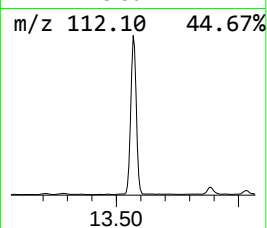
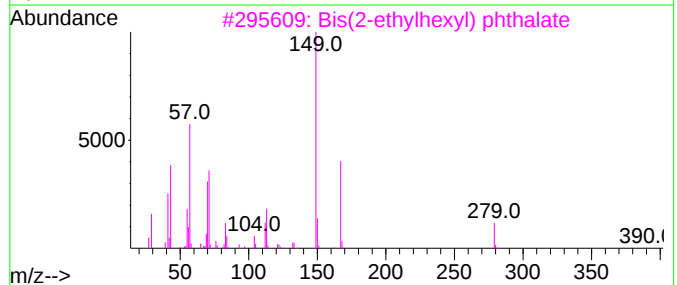
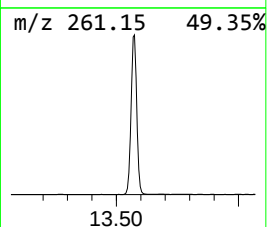
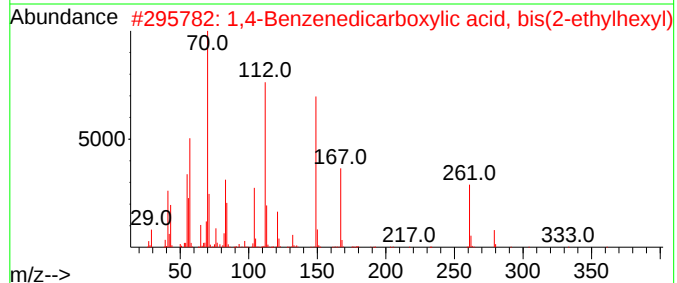
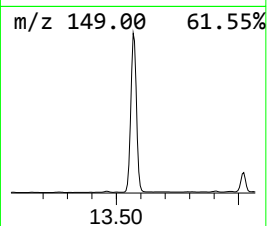
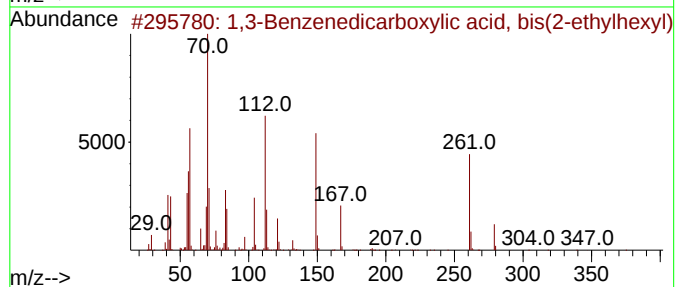
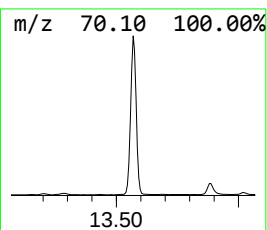
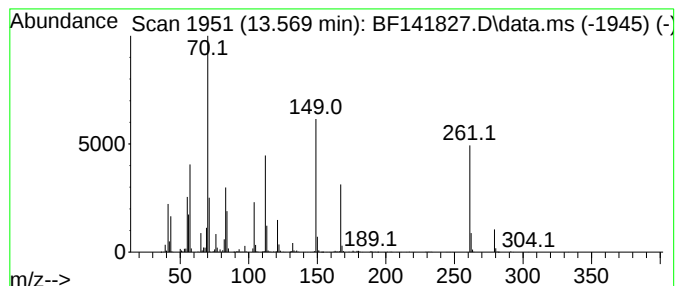
Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.569	23.20 ng	1953260	Chrysene-d12	14.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	80
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	58
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	22
4	Phthalic acid, 3,5-difluoropheny...	348	C19H18F2O4	1000315-54-1	14
5	Cyclohexanamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030425\
Data File : BF141827.D
Acq On : 04 Mar 2025 15:19
Operator : RC/JU
Sample : Q1480-25
Misc :
ALS Vial : 5 Sample Multiplier: 1

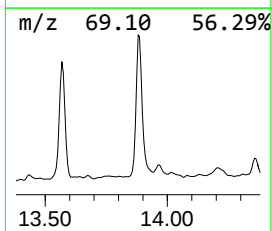
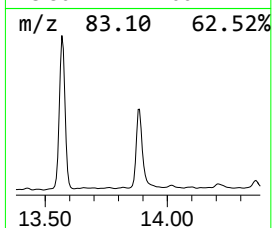
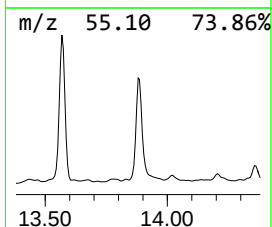
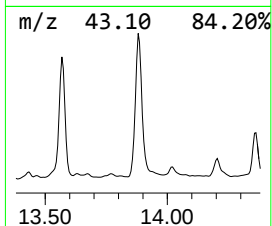
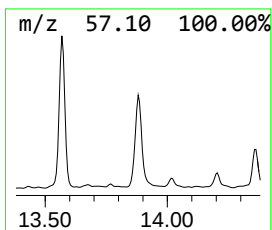
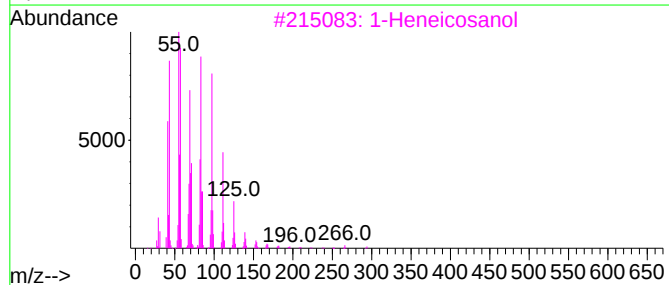
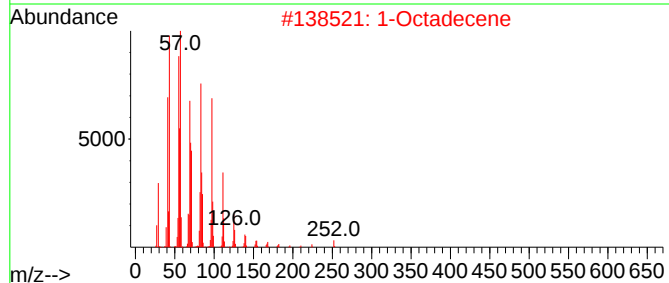
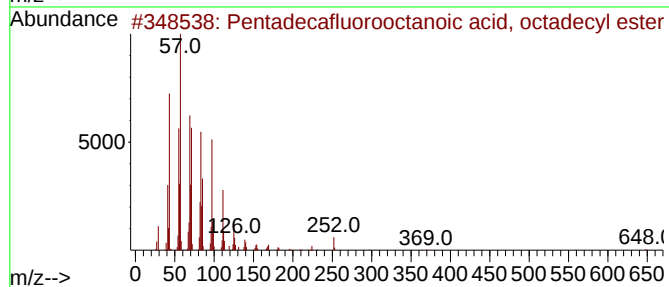
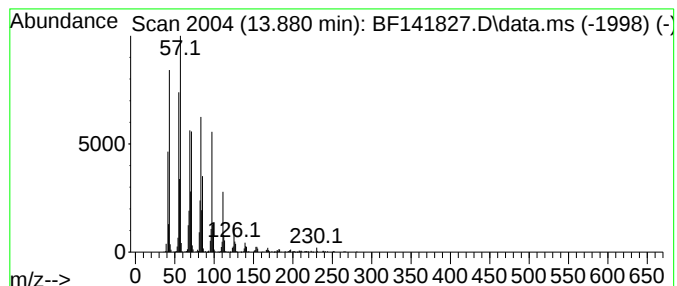
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.880	9.23 ng	777014	Chrysene-d12	14.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	1-Octadecene	252	C18H36	000112-88-9	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030425\
Data File : BF141827.D
Acq On : 04 Mar 2025 15:19
Operator : RC/JU
Sample : Q1480-25
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

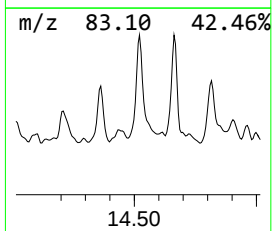
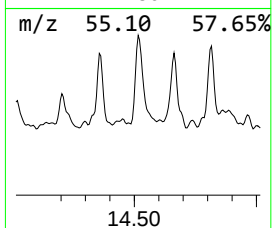
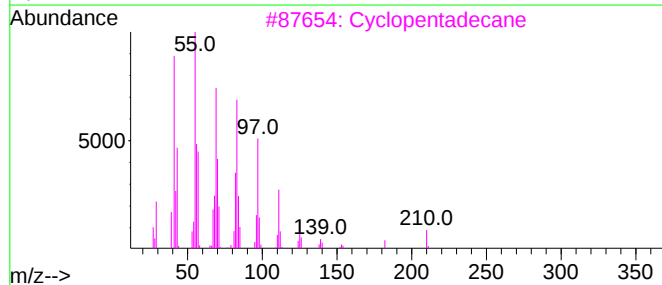
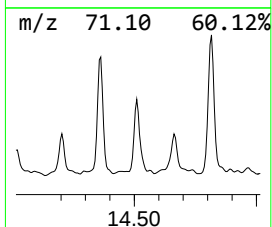
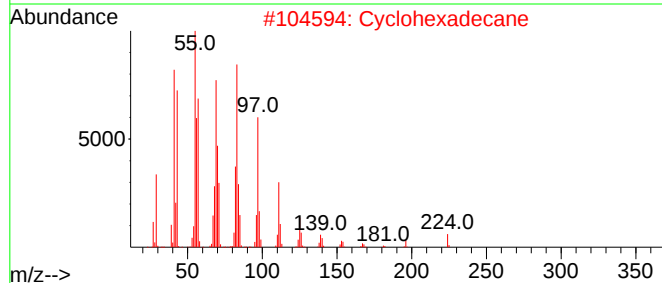
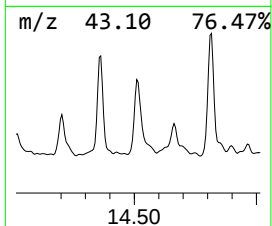
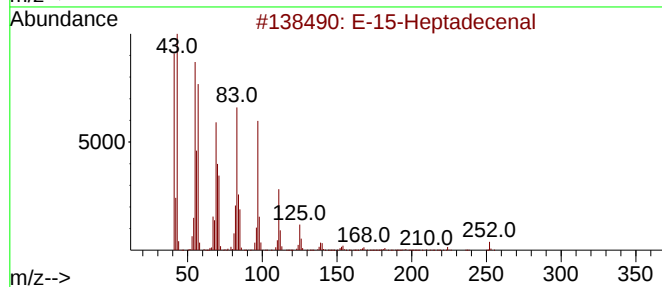
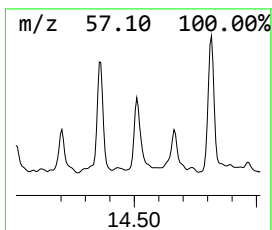
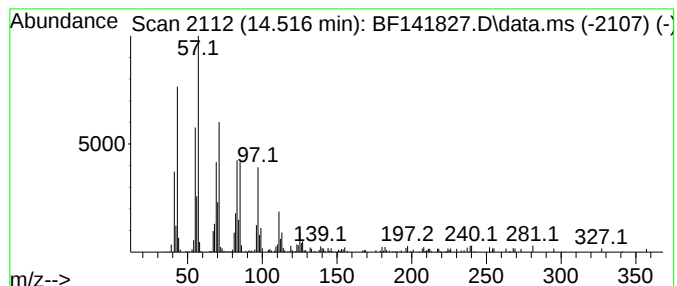
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 E-15-Heptadecenal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	2.19 ng	184193	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
2			Cyclohexadecane	224	C16H32	000295-65-8	95
3			Cyclopentadecane	210	C15H30	000295-48-7	92
4			Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	90
5			Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030425\
Data File : BF141827.D
Acq On : 04 Mar 2025 15:19
Operator : RC/JU
Sample : Q1480-25
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

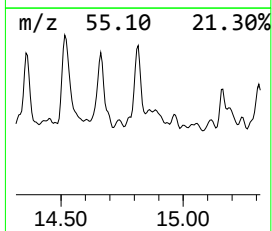
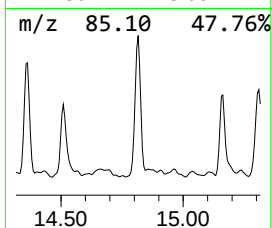
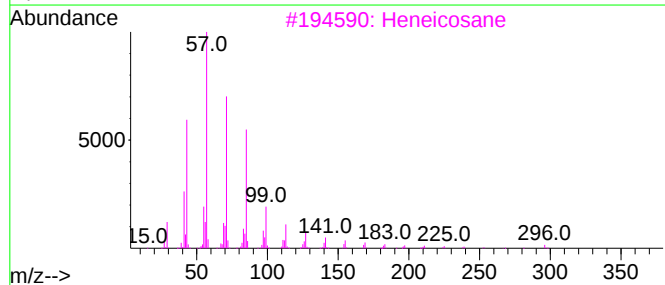
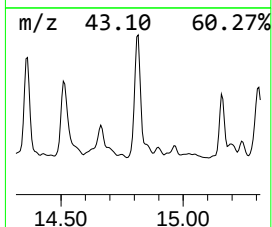
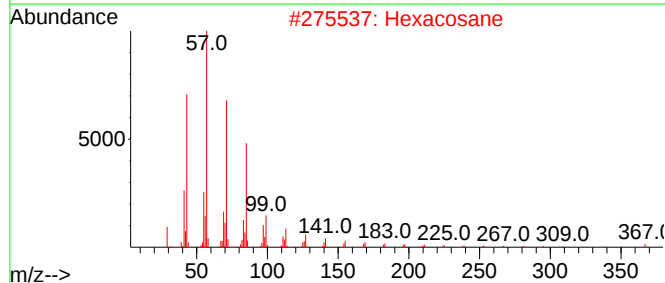
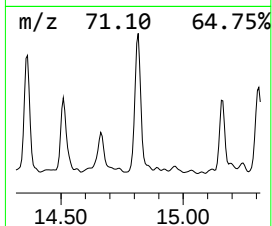
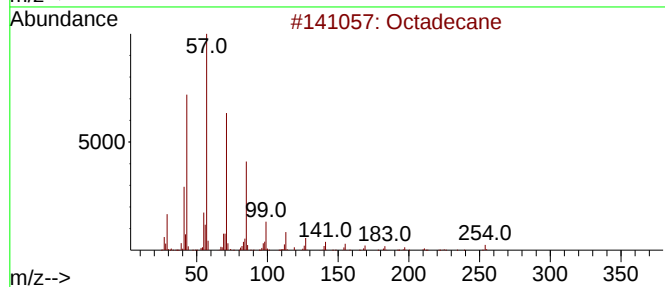
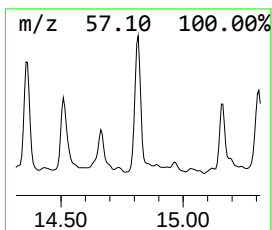
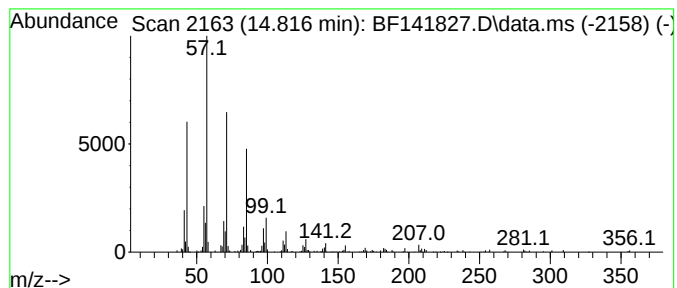
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.79 ng	193574	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030425\
Data File : BF141827.D
Acq On : 04 Mar 2025 15:19
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Sample : Q1480-25
Misc :
ALS Vial : 5 Sample Multiplier: 1

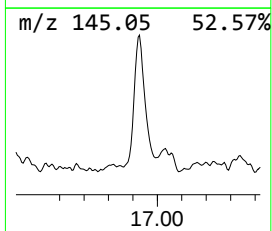
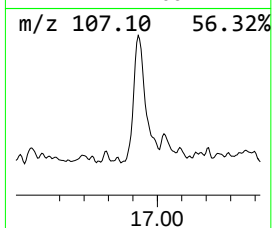
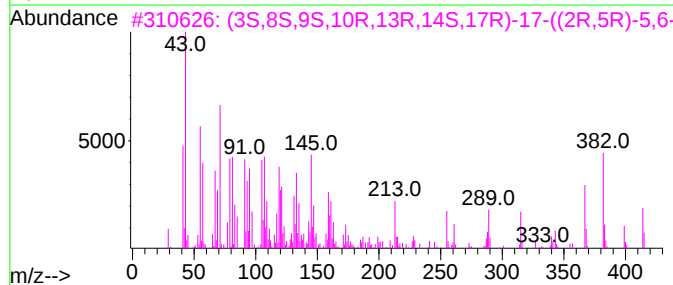
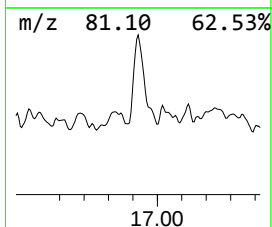
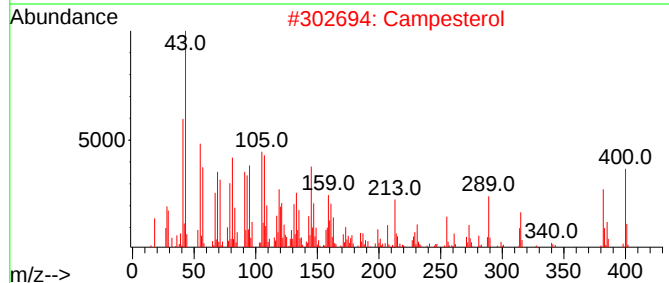
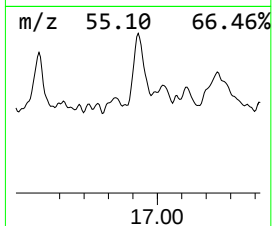
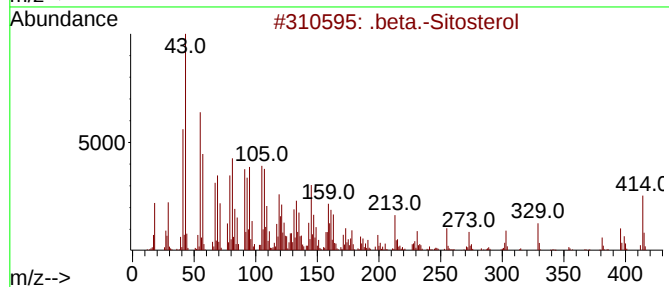
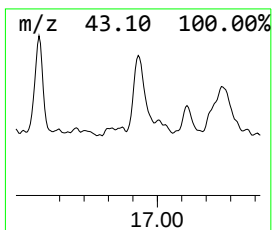
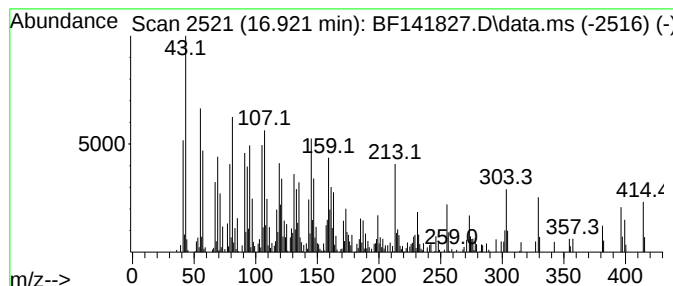
Instrument :
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ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .beta.-Sitosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.921	4.04 ng	280286	Perylene-d12	15.510	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	97
2	Campesterol	400	C28H48O	000474-62-4	59
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	55
4	Stigmasta-3,5-diene	396	C29H48	004970-37-0	46
5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030425\
Data File : BF141827.D
Acq On : 04 Mar 2025 15:19
Operator : RC/JU
Sample : Q1480-25
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.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
Butane, 2-metho...	2.228	41.3	ng	3235830	1	6.887	1566420	20.0
Benzophenone	10.628	7.6	ng	900924	3	9.916	2358480	20.0
n-Hexadecanoic ...	11.928	27.5	ng	3085260	4	11.404	2243970	20.0
Isopropyl palmi...	12.180	2.3	ng	260540	4	11.404	2243970	20.0
Octadecanoic acid	12.710	15.1	ng	1694070	4	11.404	2243970	20.0
1,3-Benzenedica...	13.569	23.2	ng	1953260	5	14.033	1684160	20.0
Pentadecafluoro...	13.880	9.2	ng	777014	5	14.033	1684160	20.0
E-15-Heptadecenal	14.515	2.2	ng	184193	5	14.033	1684160	20.0
Octadecane	14.816	2.8	ng	193574	6	15.510	1387360	20.0
.beta.-Sitosterol	16.921	4.0	ng	280286	6	15.510	1387360	20.0