

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
 Data File : BF141915.D
 Acq On : 11 Mar 2025 14:26
 Operator : RC/JU
 Sample : Q1514-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ENV-103-SB01

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-BF031025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141915.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	4	11	47	rVB	902161	1644492	36.09%	3.883%
2	5.492	572	578	597	rBV	2050013	2742709	60.19%	6.476%
3	6.498	742	749	761	rBV	1979535	2806861	61.60%	6.628%
4	6.881	808	814	819	rBV	716657	910527	19.98%	2.150%
5	7.434	902	908	914	rBV	1415872	1893267	41.55%	4.470%
6	7.686	946	951	958	rBV	53256	67470	1.48%	0.159%
7	8.157	1026	1031	1040	rBV	981458	1238574	27.18%	2.925%
8	9.233	1208	1214	1219	rBV	3193412	3995772	87.69%	9.435%
9	9.910	1324	1329	1334	rBV	1181179	1488984	32.68%	3.516%
10	10.622	1445	1450	1455	rBV	409166	515356	11.31%	1.217%
11	10.698	1457	1463	1475	rBV	2150339	2746486	60.27%	6.485%
12	11.398	1577	1582	1590	rBV2	1238546	1772966	38.91%	4.186%
13	11.851	1654	1659	1660	rVV2	34167	58319	1.28%	0.138%
14	11.921	1661	1671	1683	rVV	1202517	2517203	55.24%	5.944%
15	12.010	1683	1686	1693	rVV	57285	113655	2.49%	0.268%
16	12.080	1694	1698	1705	rVB6	23454	48218	1.06%	0.114%
17	12.292	1721	1734	1750	rVB	1434236	4556693	100.00%	10.759%
18	12.439	1754	1759	1763	rBV3	61933	93641	2.06%	0.221%
19	12.610	1784	1788	1795	rVV	275720	523198	11.48%	1.235%
20	12.704	1796	1804	1818	rVV	1576896	3205032	70.34%	7.568%
21	12.839	1822	1827	1842	rVB	219574	475117	10.43%	1.122%
22	12.986	1846	1852	1857	rVB	3373523	4448617	97.63%	10.504%
23	13.163	1876	1882	1886	rVB2	29937	57324	1.26%	0.135%
24	13.227	1888	1893	1897	rBV3	34622	67906	1.49%	0.160%
25	13.674	1962	1969	1978	rVB3	82718	220941	4.85%	0.522%
26	13.904	2001	2008	2022	rBV5	123709	422434	9.27%	0.997%
27	14.033	2024	2030	2040	rVB	995436	1435243	31.50%	3.389%
28	14.198	2055	2058	2063	rVB	42037	54055	1.19%	0.128%
29	14.298	2070	2075	2080	rBV	68981	122483	2.69%	0.289%
30	14.504	2106	2110	2114	rBV	74700	103921	2.28%	0.245%
31	14.662	2133	2137	2145	rVB	62224	97681	2.14%	0.231%
32	14.815	2158	2163	2172	rBV	122025	241512	5.30%	0.570%
33	14.892	2173	2176	2182	rVB	45671	60407	1.33%	0.143%
34	15.074	2203	2207	2215	rVB	65123	137581	3.02%	0.325%
35	15.157	2217	2221	2227	rBV2	80322	122613	2.69%	0.290%
36	15.380	2255	2259	2265	rBV2	44779	102787	2.26%	0.243%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.439	2266	2269	2273	rVB	45996	63380	1.39%	0.150%
38	15.504	2275	2280	2286	rBV	683932	1113863	24.44%	2.630%
39	15.986	2358	2362	2367	rVB	40275	63306	1.39%	0.149%

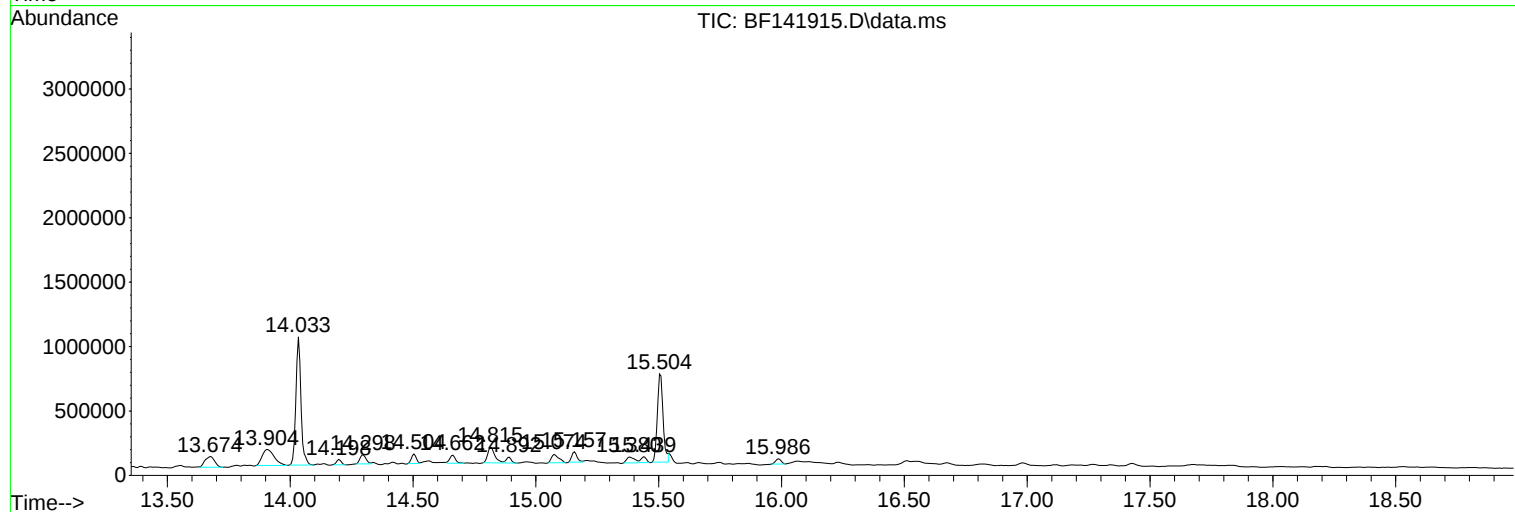
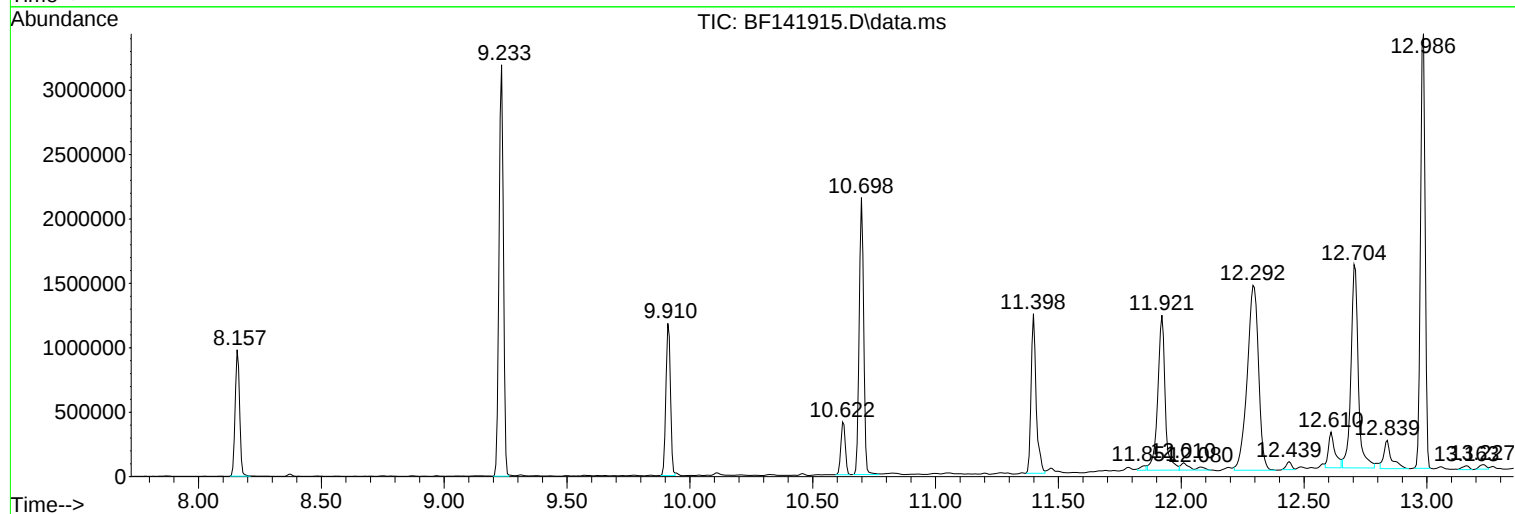
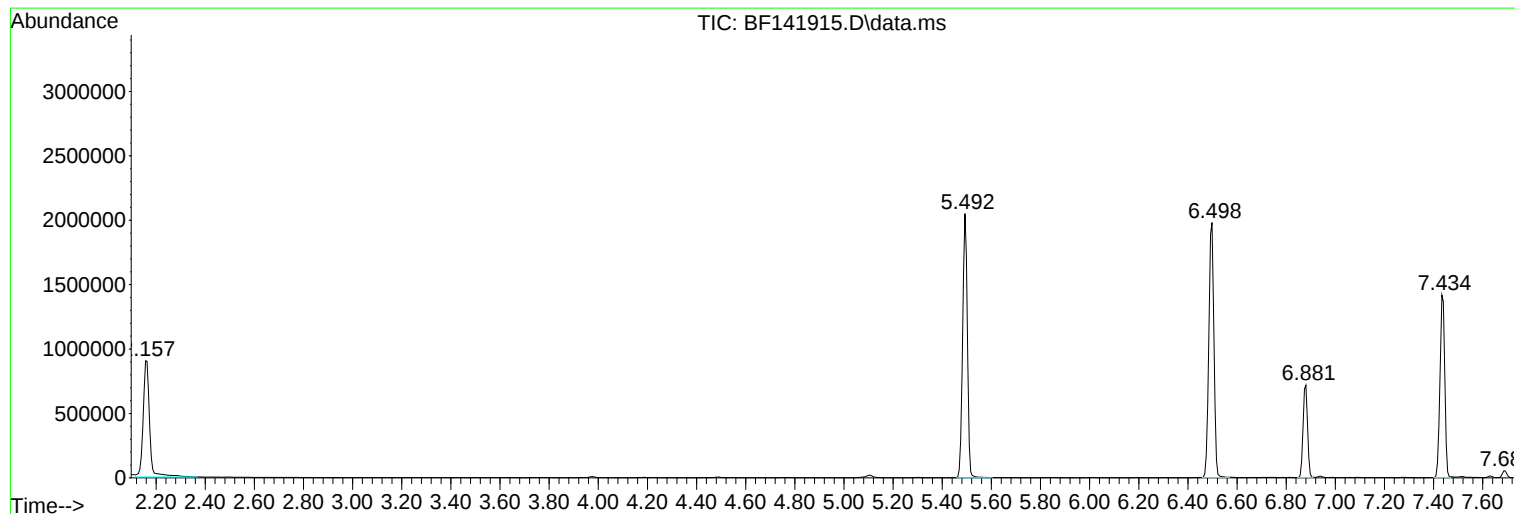
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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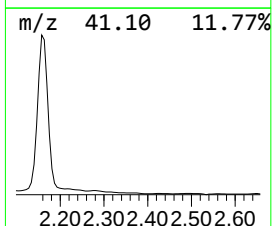
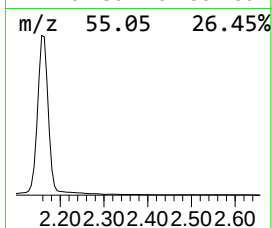
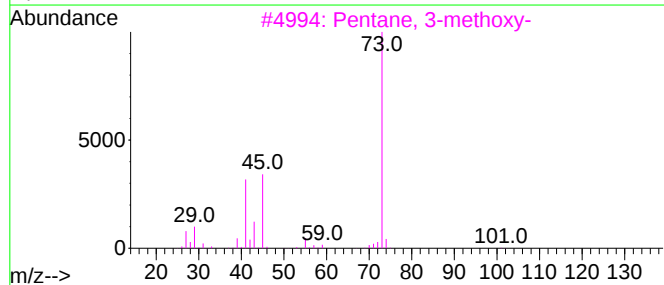
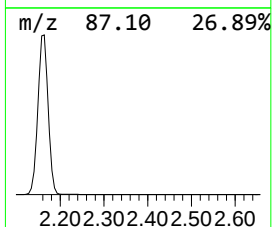
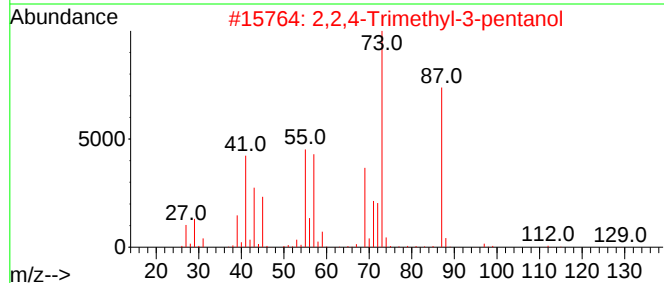
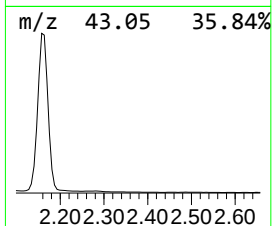
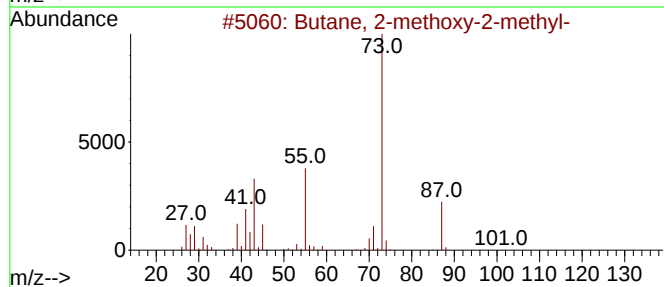
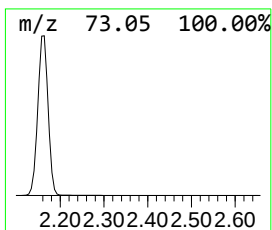
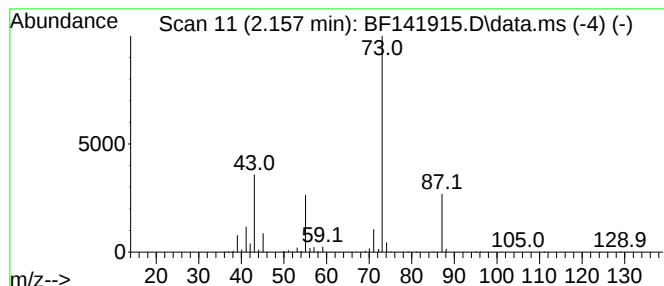
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	36.12 ng	1644490	1,4-Dichlorobenzene-d4	6.881

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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Instrument :
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ClientSampleId :
ENV-103-SB01

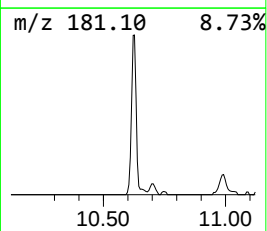
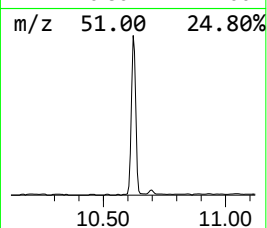
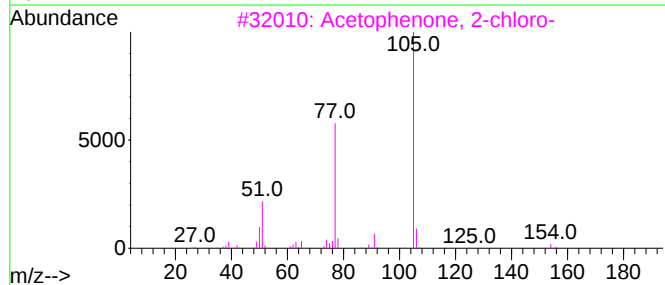
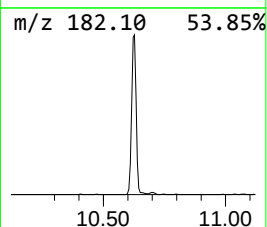
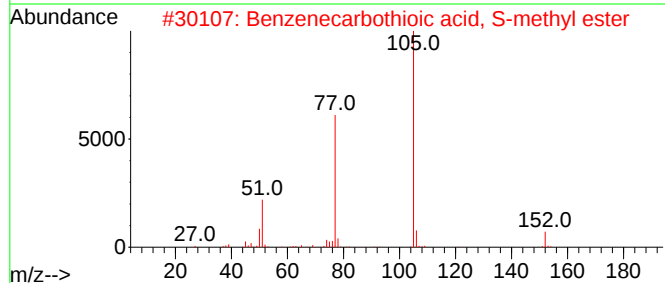
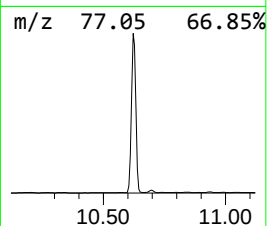
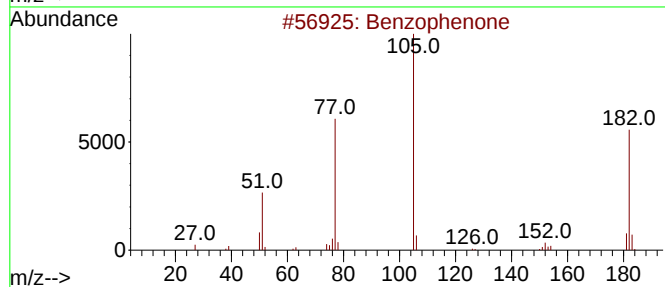
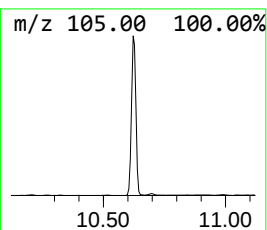
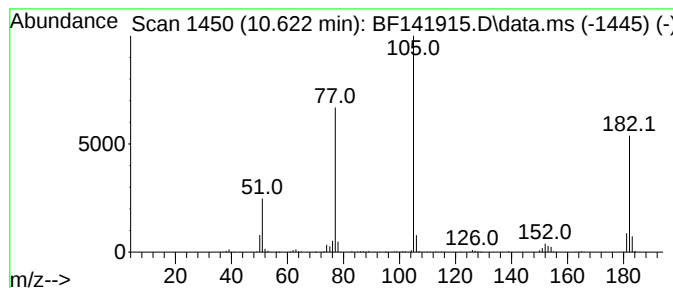
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	6.92 ng	515356	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzenecarboxylic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47



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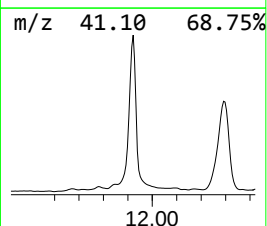
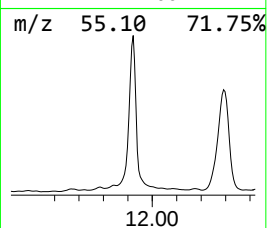
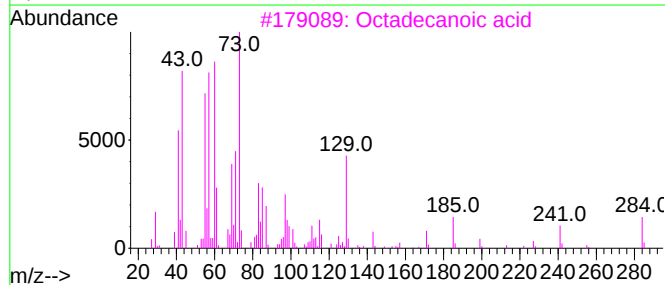
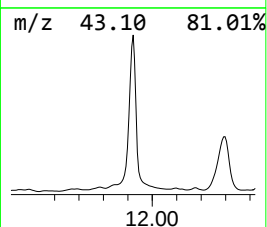
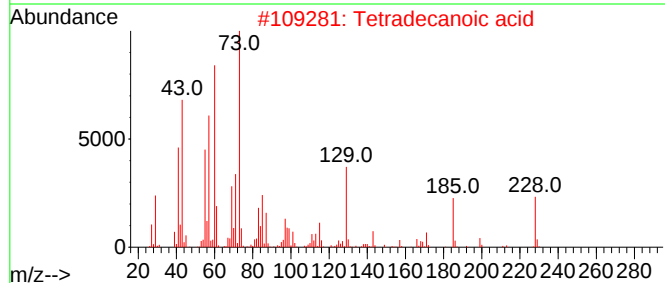
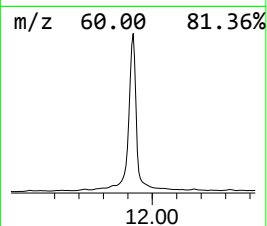
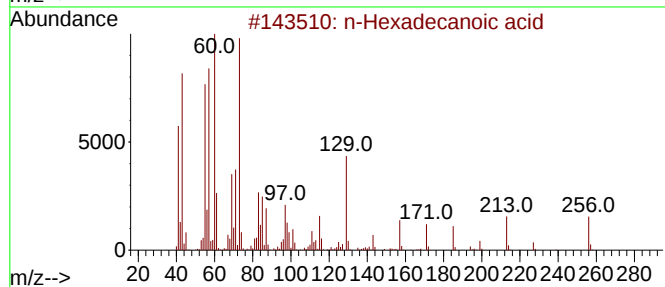
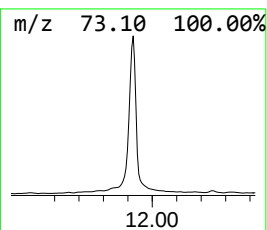
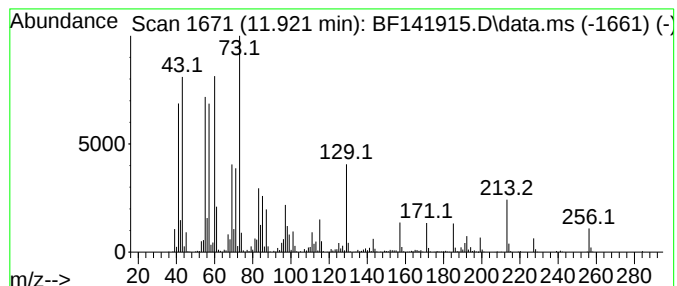
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	28.40 ng	2517200	Phenanthrene-d10	11.398

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	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	91



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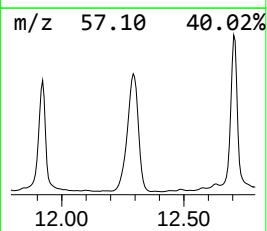
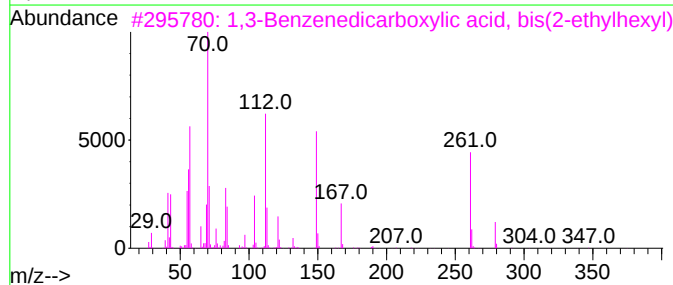
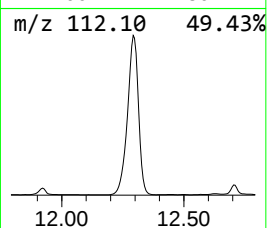
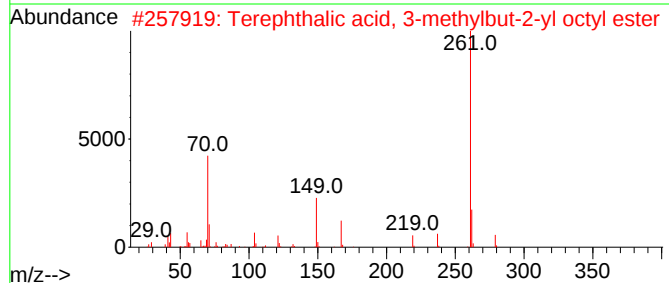
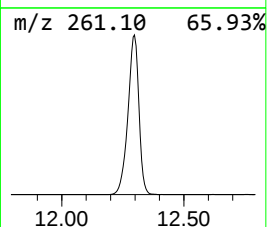
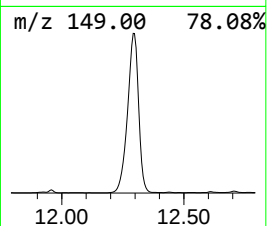
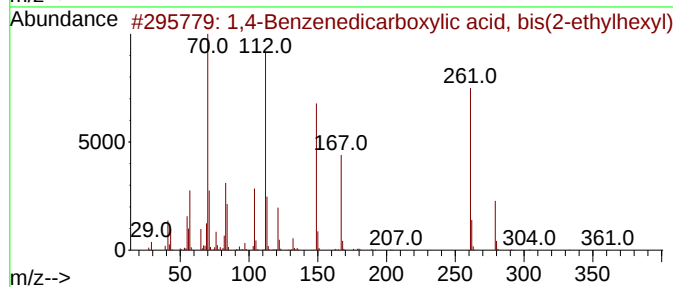
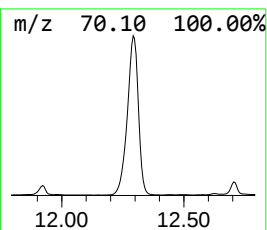
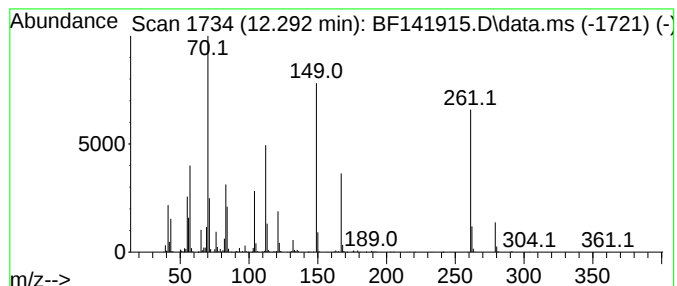
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.292	51.40 ng	4556690	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
4			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43
5			Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	38



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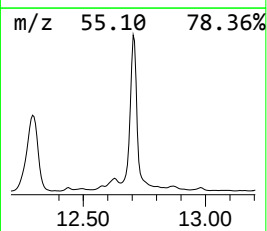
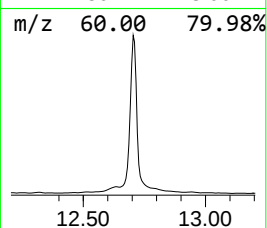
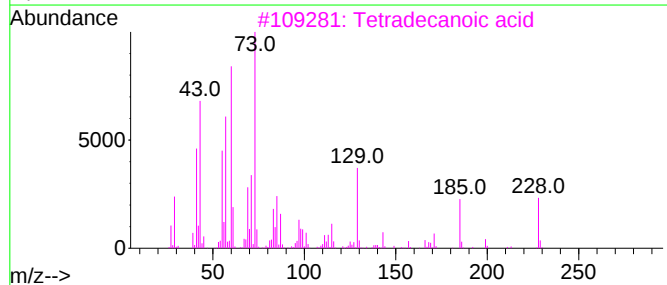
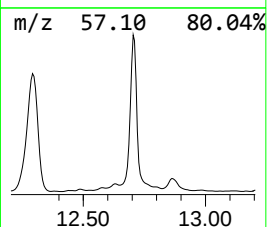
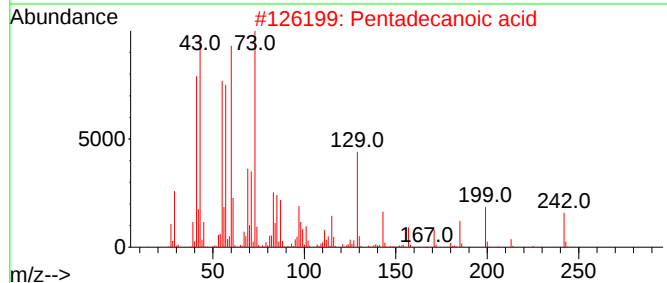
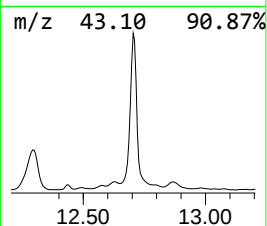
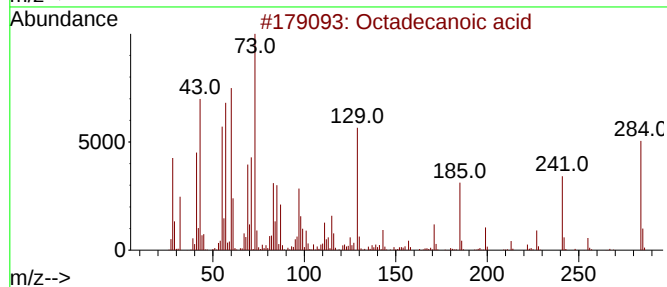
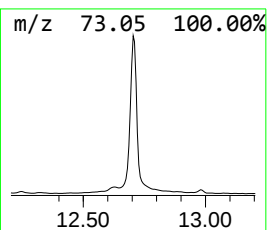
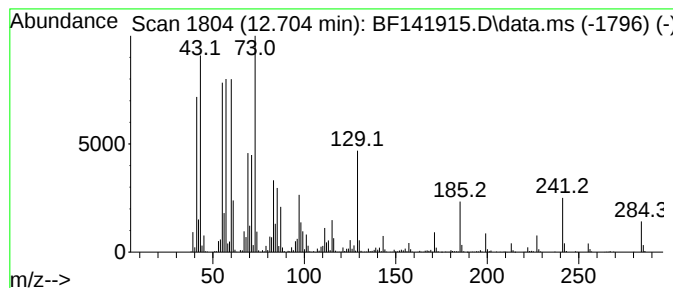
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	36.15 ng	3205030	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141915.D
Acq On : 11 Mar 2025 14:26
Operator : RC/JU
Sample : Q1514-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

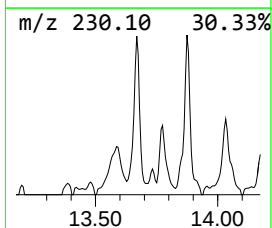
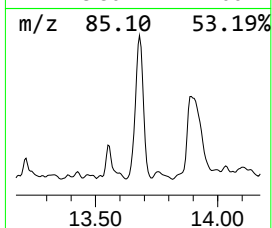
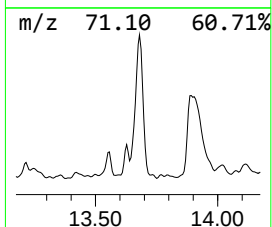
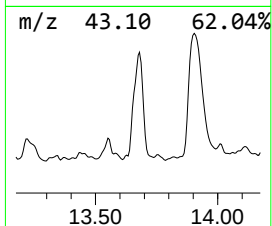
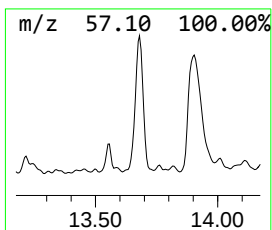
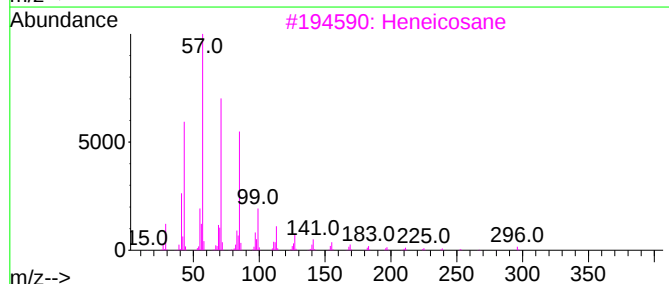
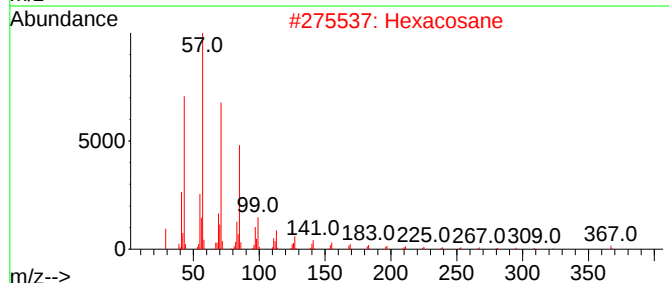
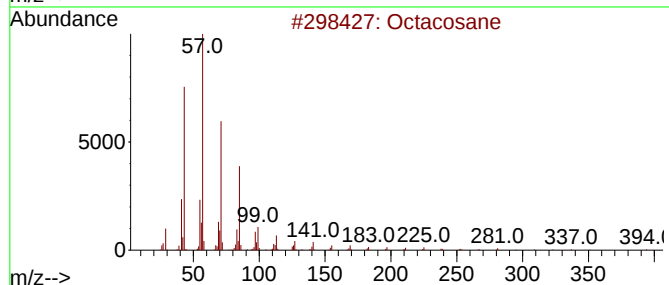
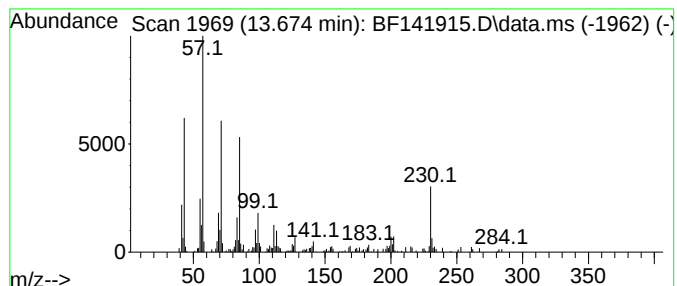
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.674	3.08 ng	220941	Chrysene-d12	14.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	76
2	Hexacosane	366	C26H54	000630-01-3	74
3	Heneicosane	296	C21H44	000629-94-7	74
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72
5	Tetratetracontane	619	C44H90	007098-22-8	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141915.D
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Sample : Q1514-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

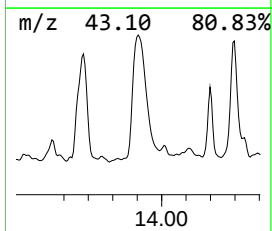
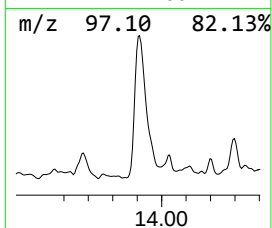
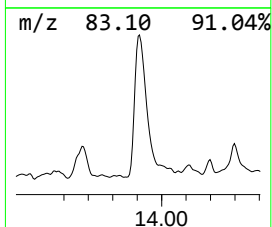
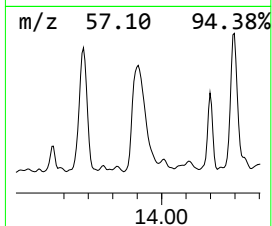
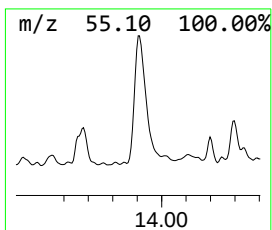
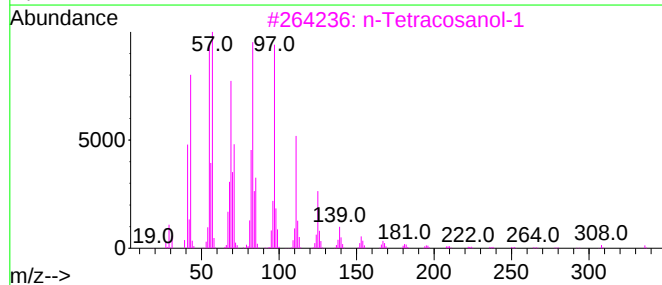
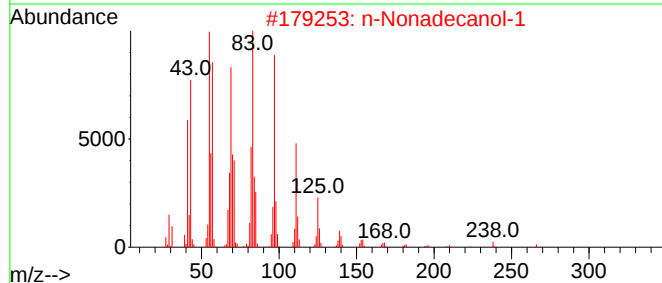
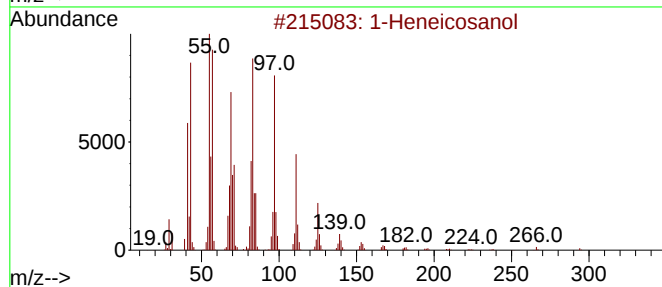
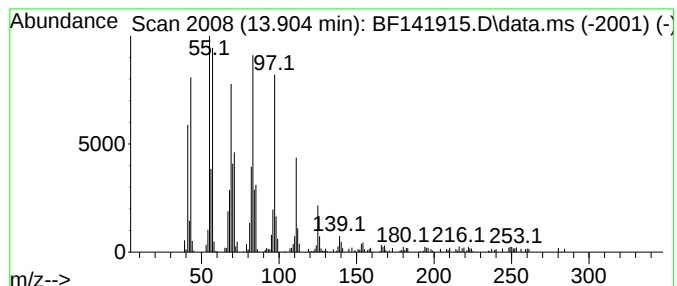
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.904	5.89 ng	422434	Chrysene-d12	14.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141915.D
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Operator : RC/JU
Sample : Q1514-05
Misc :
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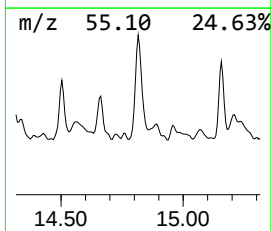
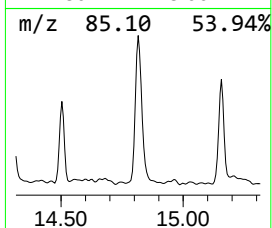
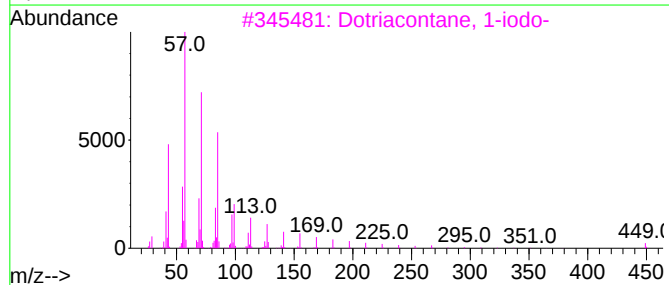
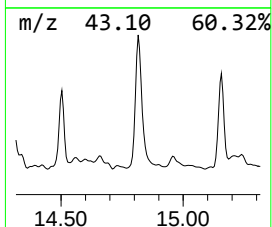
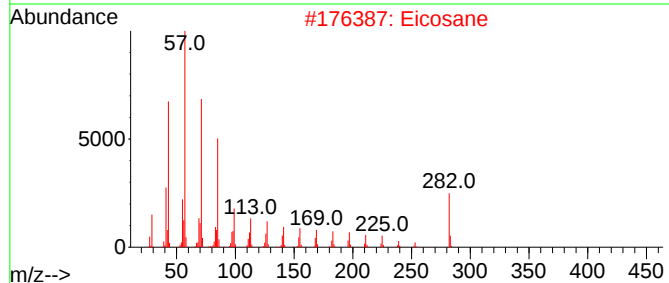
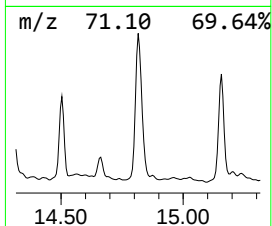
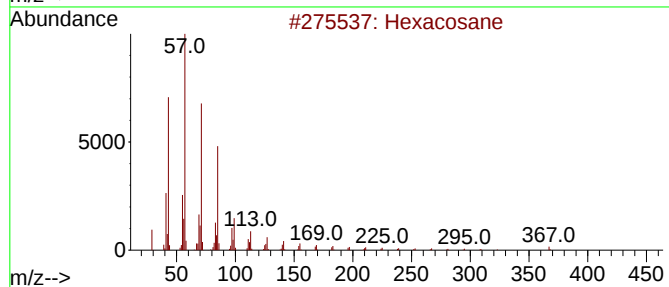
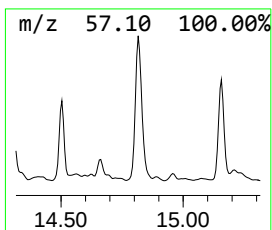
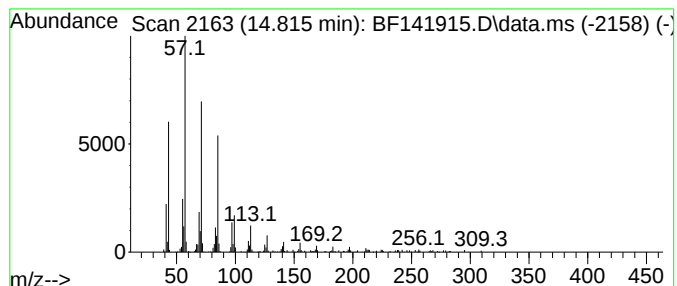
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.815	4.34 ng	241512	Perylene-d12		15.504	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	94
2	Eicosane		282	C20H42	000112-95-8	93
3	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	90
4	Heneicosane		296	C21H44	000629-94-7	90
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141915.D
Acq On : 11 Mar 2025 14:26
Operator : RC/JU
Sample : Q1514-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

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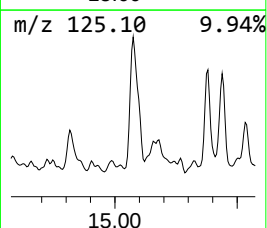
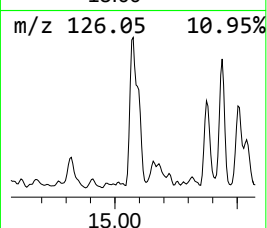
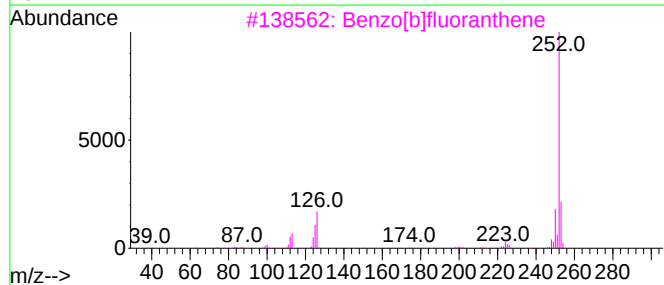
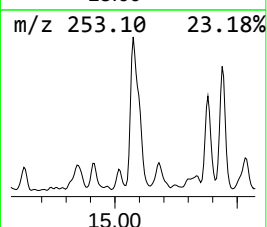
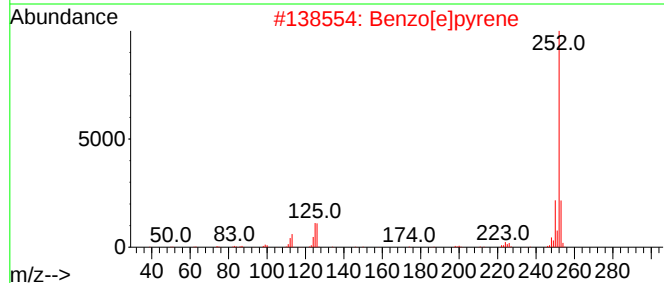
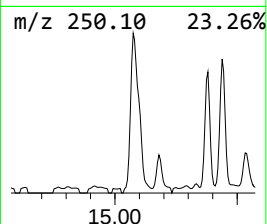
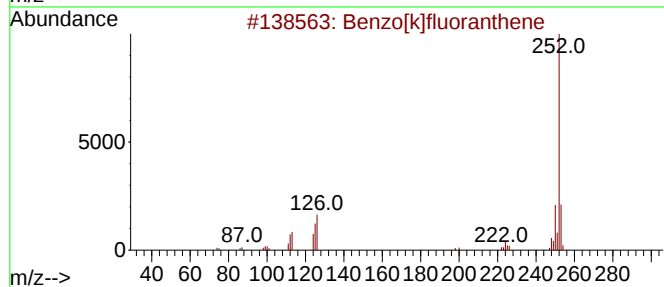
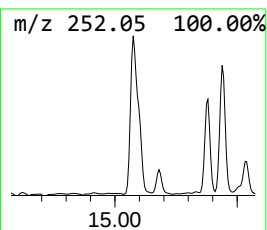
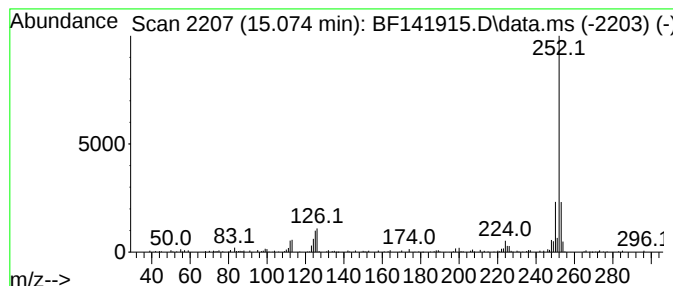
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	2.47 ng	137581	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2			Benzo[e]pyrene	252	C20H12	000192-97-2	96
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4			Benzo[a]pyrene	252	C20H12	000050-32-8	94
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141915.D
Acq On : 11 Mar 2025 14:26
Operator : RC/JU
Sample : Q1514-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ENV-103-SB01

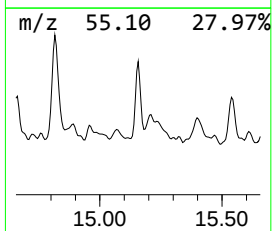
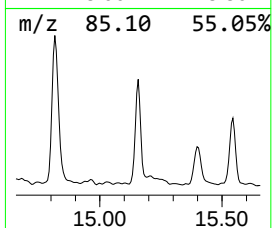
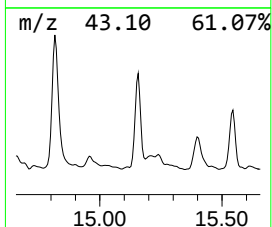
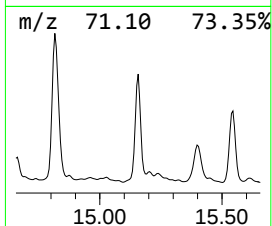
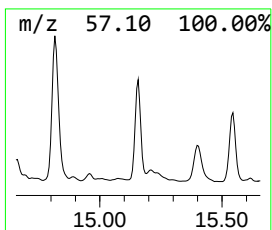
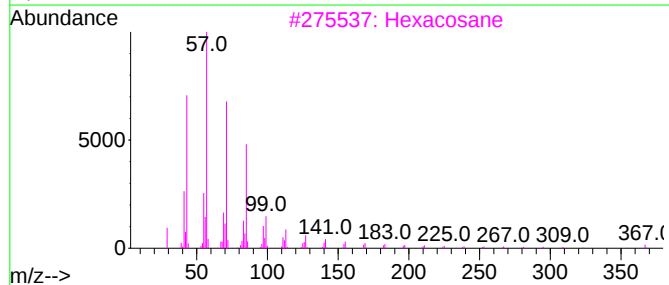
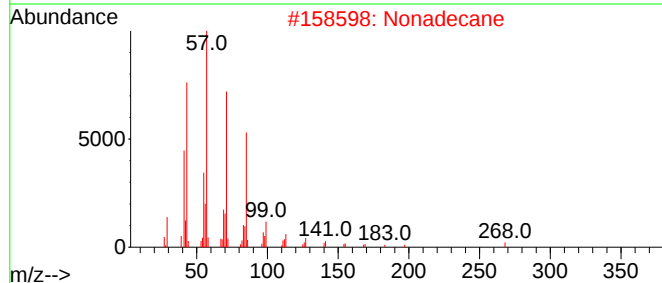
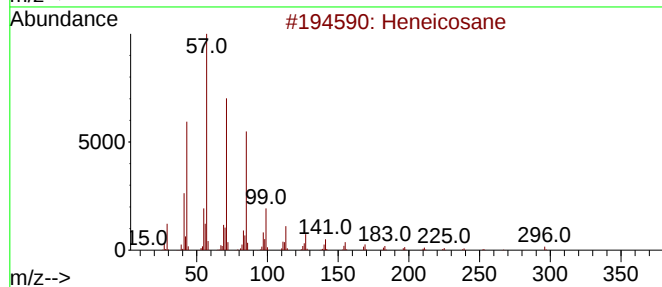
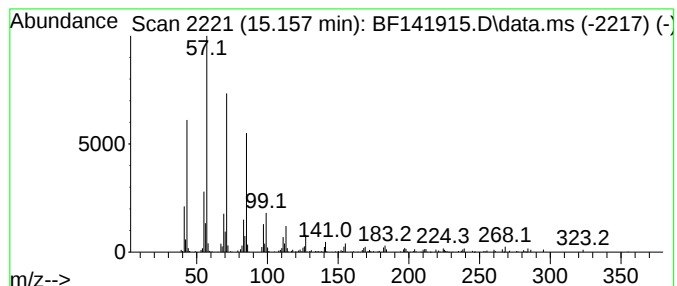
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.157	2.20 ng	122613	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Nonadecane	268	C19H40	000629-92-5	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031125\
Data File : BF141915.D
Acq On : 11 Mar 2025 14:26
Operator : RC/JU
Sample : Q1514-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-103-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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	10.622	6.9	ng	515356	3	9.910	1488980	20.0
n-Hexadecanoic ...	11.922	28.4	ng	2517200	4	11.398	1772970	20.0
1,4-Benzenedica...	12.292	51.4	ng	4556690	4	11.398	1772970	20.0
Octadecanoic acid	12.704	36.1	ng	3205030	4	11.398	1772970	20.0
Octacosane	13.674	3.1	ng	220941	5	14.033	1435240	20.0
1-Heneicosanol	13.904	5.9	ng	422434	5	14.033	1435240	20.0
Hexacosane	14.815	4.3	ng	241512	6	15.504	1113860	20.0
Benzo[e]pyrene	15.074	2.5	ng	137581	6	15.504	1113860	20.0
Heneicosane	15.157	2.2	ng	122613	6	15.504	1113860	20.0