

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
 Data File : BF140525.D
 Acq On : 21 Nov 2024 02:35
 Operator : RC/JU
 Sample : P4916-05
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2-WC

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-BF111324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	5	23	rVB	403819	531083	43.14%	4.976%
2	5.504	574	580	598	rVB	733326	983747	79.91%	9.217%
3	6.510	746	751	767	rBV	699734	929802	75.52%	8.712%
4	6.875	808	813	820	rBV	320511	390063	31.68%	3.655%
5	7.434	902	908	918	rBV	440862	570358	46.33%	5.344%
6	7.687	946	951	962	rVB2	10089	19352	1.57%	0.181%
7	8.151	1023	1030	1046	rVB	320780	429831	34.91%	4.027%
8	9.228	1207	1213	1222	rBV	788713	1034078	83.99%	9.689%
9	9.298	1222	1225	1236	rVB3	7913	16244	1.32%	0.152%
10	9.769	1301	1305	1312	rBV	16200	22915	1.86%	0.215%
11	9.910	1323	1329	1339	rBV	350740	453242	36.82%	4.247%
12	9.998	1339	1344	1352	rVV	147551	230271	18.70%	2.158%
13	10.333	1393	1401	1404	rBV4	9176	15857	1.29%	0.149%
14	10.622	1444	1450	1458	rBV	159580	212133	17.23%	1.988%
15	10.698	1458	1463	1474	rVV	474998	641125	52.08%	6.007%
16	10.810	1478	1482	1488	rVB3	14787	27712	2.25%	0.260%
17	10.928	1499	1502	1507	rVB	17218	22491	1.83%	0.211%
18	11.251	1554	1557	1560	rBV2	10661	14317	1.16%	0.134%
19	11.286	1560	1563	1568	rVB3	10363	16589	1.35%	0.155%
20	11.398	1577	1582	1591	rBV2	409848	596433	48.45%	5.588%
21	11.475	1591	1595	1598	rVV	13348	18494	1.50%	0.173%
22	11.680	1626	1630	1634	rVV2	16534	22690	1.84%	0.213%
23	11.733	1635	1639	1644	rVB	11188	17553	1.43%	0.164%
24	11.922	1663	1671	1677	rBV4	85649	184471	14.98%	1.728%
25	12.010	1683	1686	1695	rVB2	40195	84826	6.89%	0.795%
26	12.086	1695	1699	1704	rBV3	25872	37379	3.04%	0.350%
27	12.198	1715	1718	1720	rBV2	10749	13560	1.10%	0.127%
28	12.333	1737	1741	1745	rBV4	15451	30407	2.47%	0.285%
29	12.375	1745	1748	1751	rBV2	17286	21985	1.79%	0.206%
30	12.451	1757	1761	1763	rBV	37144	47755	3.88%	0.447%
31	12.480	1763	1766	1773	rVB3	46613	68114	5.53%	0.638%
32	12.539	1773	1776	1779	rBV2	14442	20199	1.64%	0.189%
33	12.616	1785	1789	1794	rBV	142348	183665	14.92%	1.721%
34	12.716	1802	1806	1809	rBV3	18588	30329	2.46%	0.284%
35	12.845	1822	1828	1834	rBV	183887	289574	23.52%	2.713%
36	12.898	1835	1837	1841	rVB2	18375	22126	1.80%	0.207%

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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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.986	1846	1852	1860	rVB	909473	1231124	100.00%	11.535%
38	13.210	1886	1890	1893	rBV2	53462	75577	6.14%	0.708%
39	13.551	1945	1948	1952	rBV2	47479	59051	4.80%	0.553%
40	14.045	2028	2032	2043	rVB2	298362	497663	40.42%	4.663%
41	14.804	2158	2161	2168	rBV3	145024	225240	18.30%	2.110%
42	15.545	2283	2287	2296	rVB2	204939	333550	27.09%	3.125%

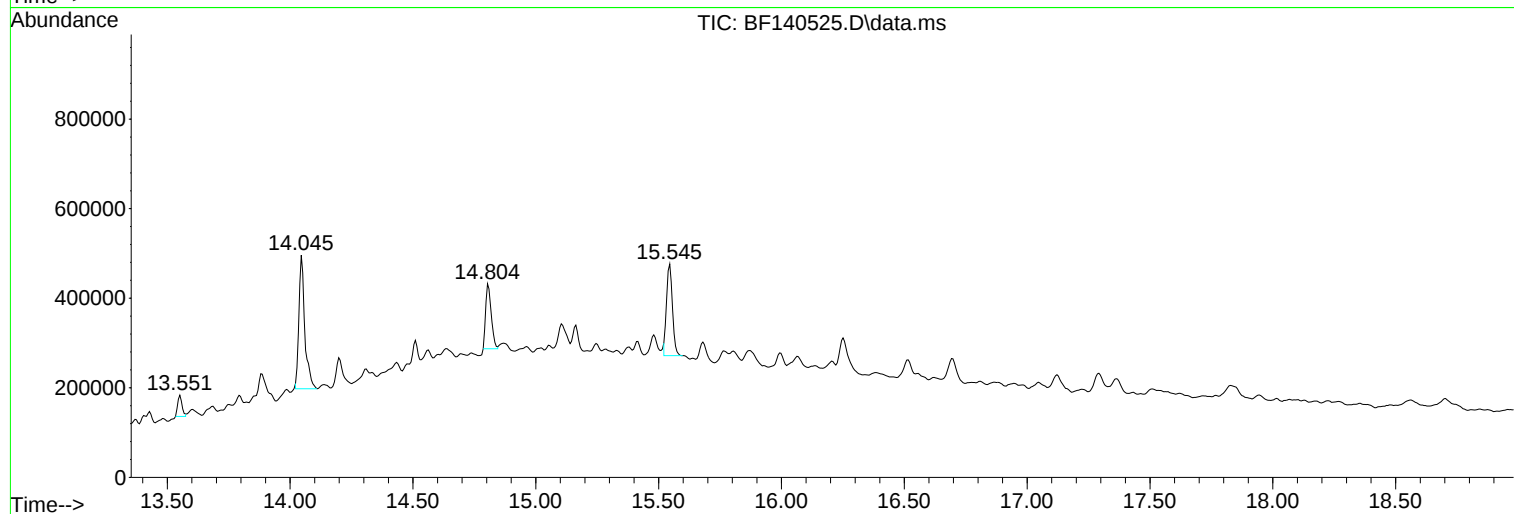
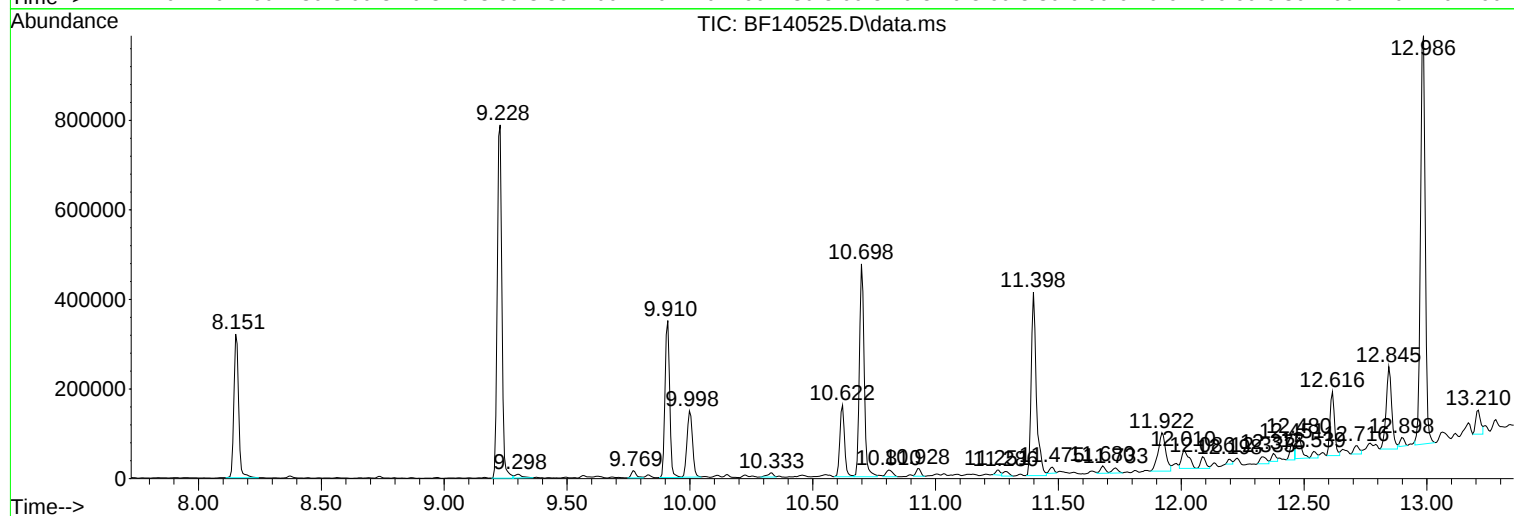
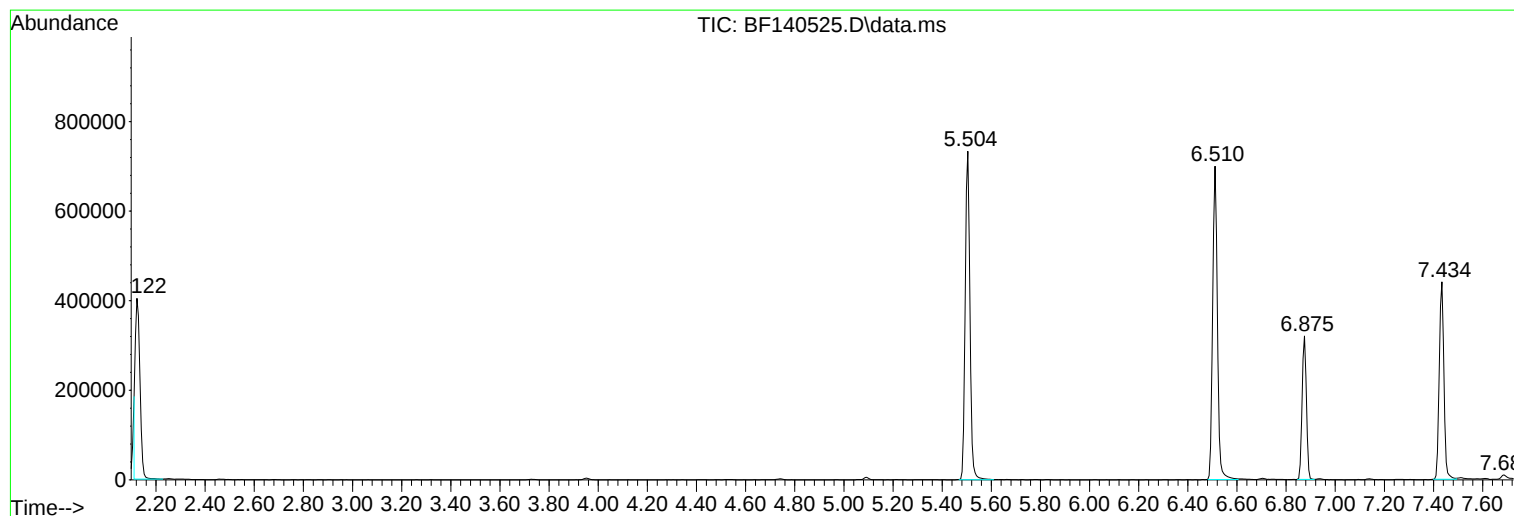
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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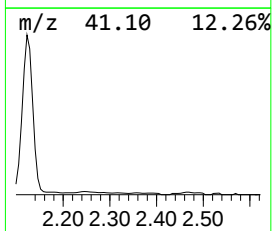
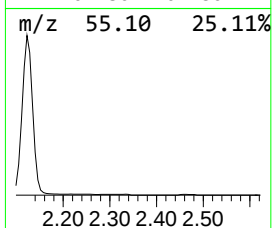
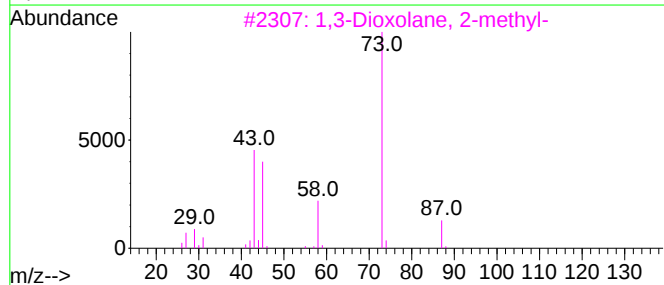
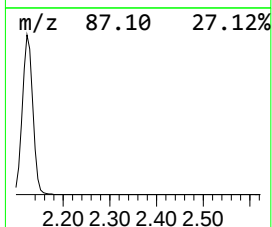
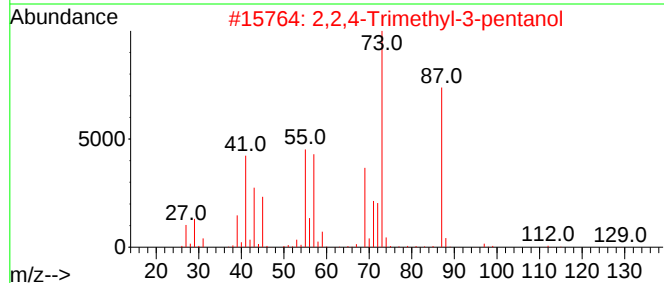
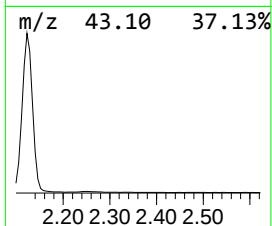
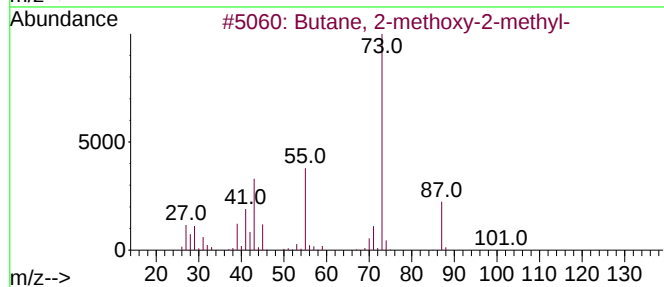
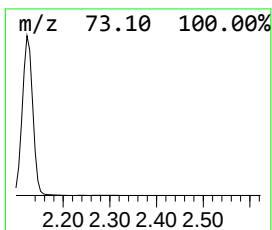
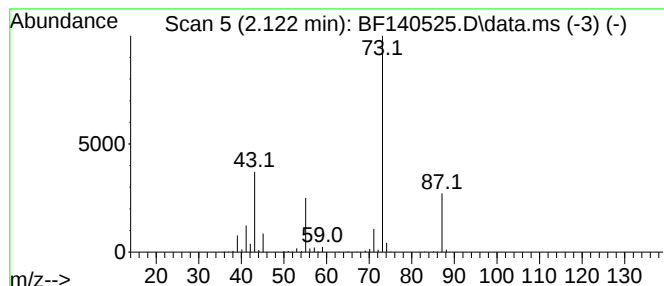
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	27.23 ng	531083	1,4-Dichlorobenzene-d4	6.875

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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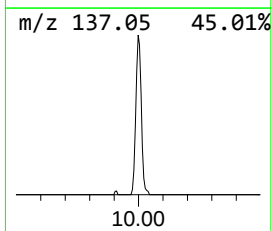
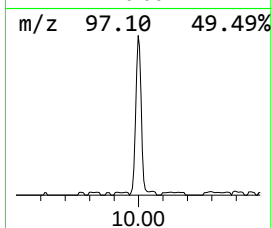
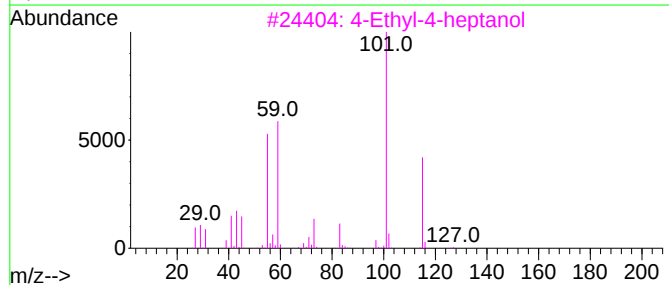
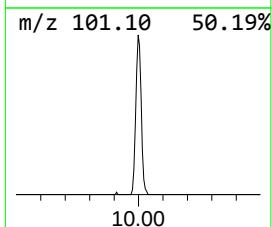
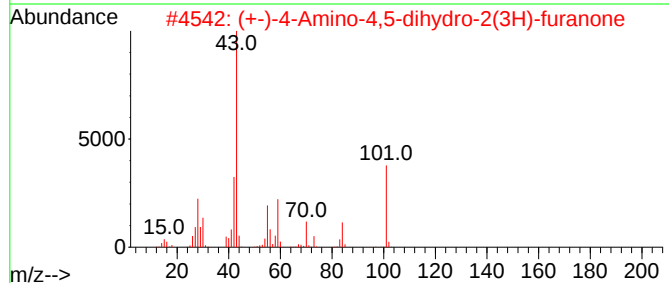
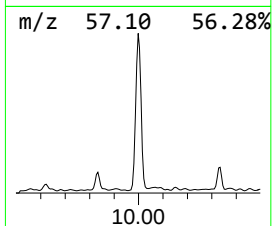
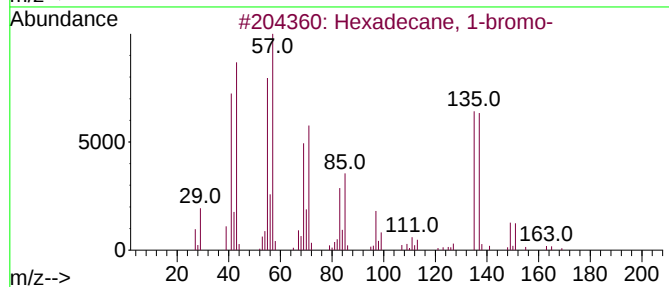
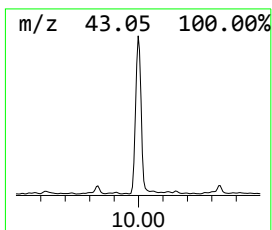
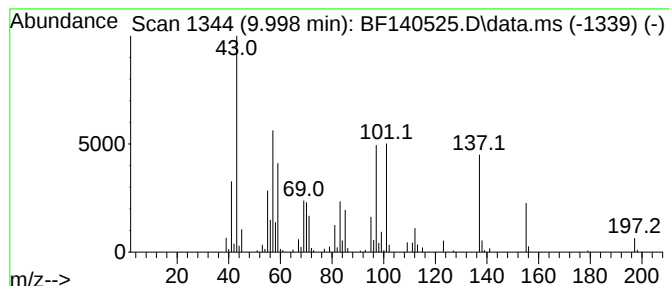
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown9.998 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	10.16 ng	230271	Acenaphthene-d10	9.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	27
2		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
3		4-Ethyl-4-heptanol	144	C9H20O	000597-90-0	22
4		trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
5		Octyl (E)-2-methylbut-2-enoate	212	C13H24O2	1000373-71-2	10



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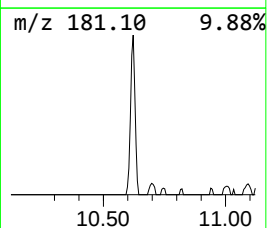
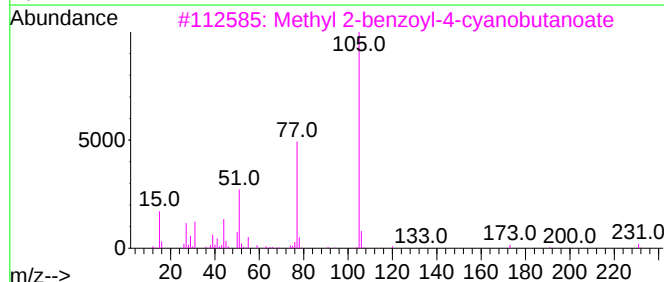
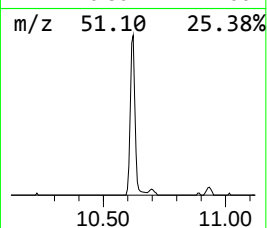
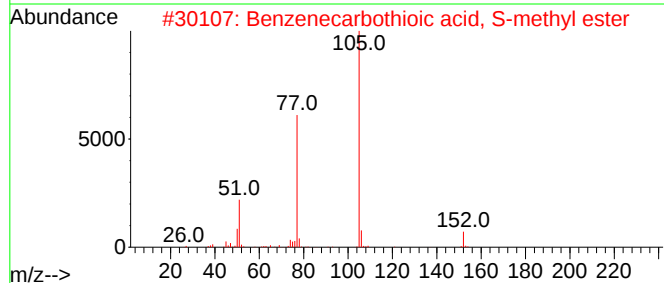
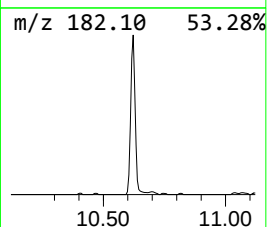
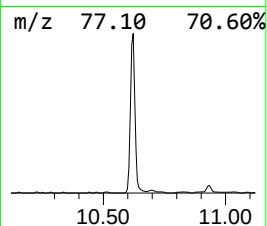
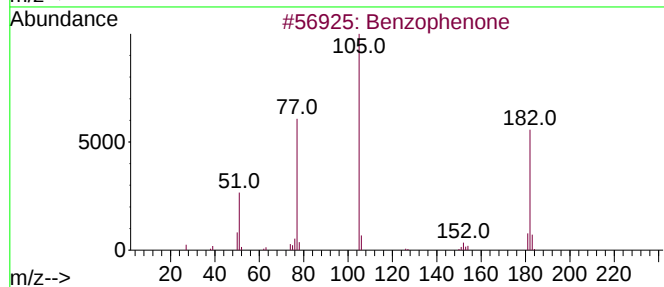
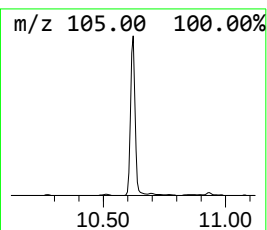
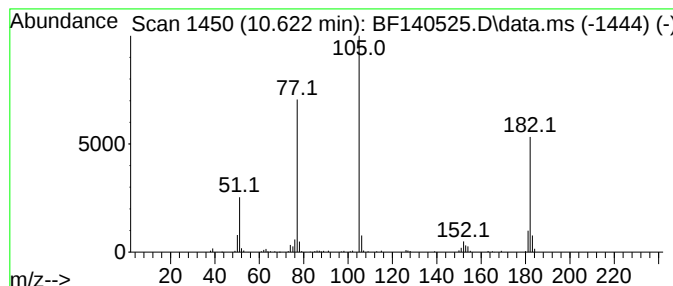
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	9.36 ng	212133	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	49
3			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
4			Benzilic acid	228	C14H12O3	000076-93-7	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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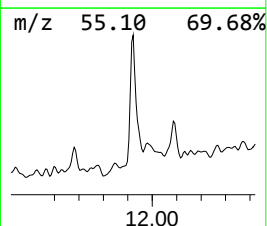
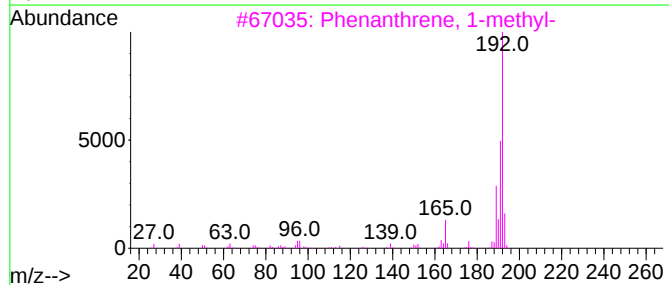
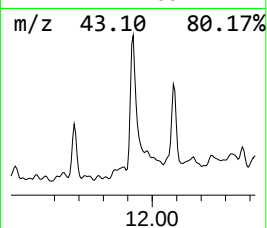
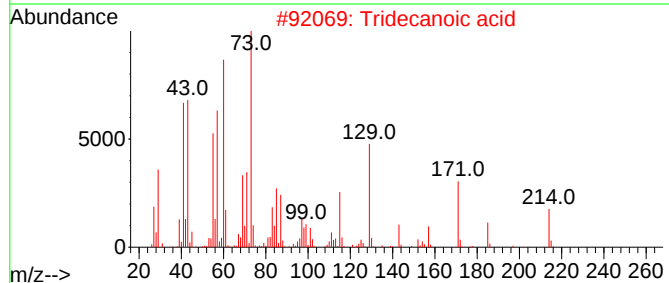
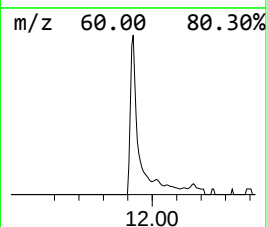
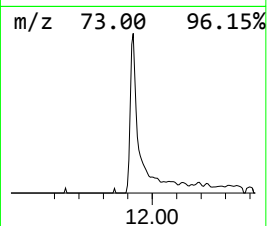
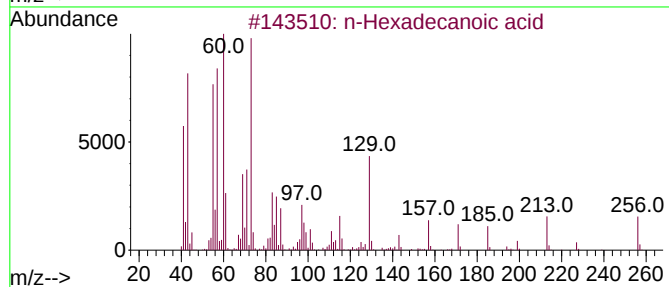
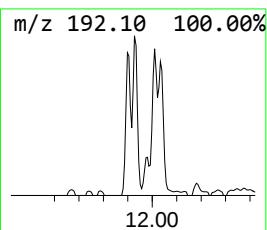
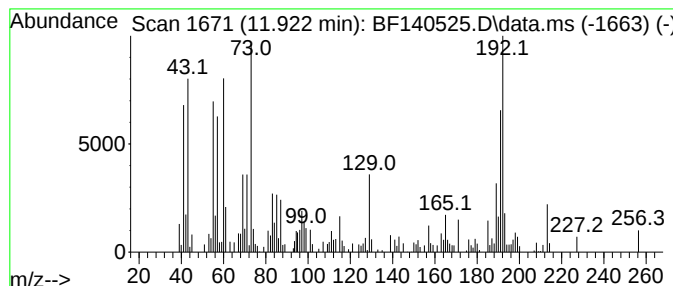
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	6.19 ng	184471	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	84
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	78
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	76



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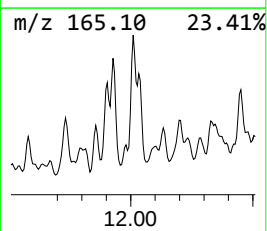
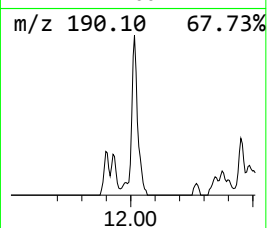
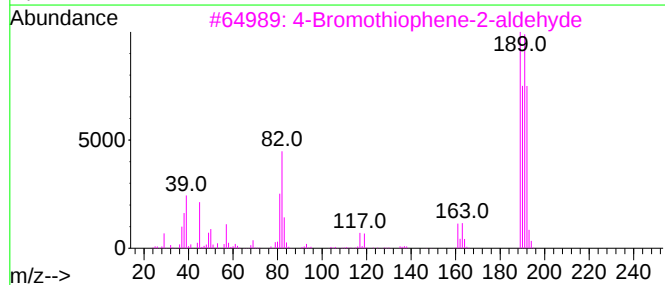
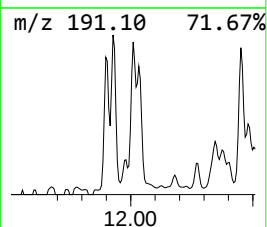
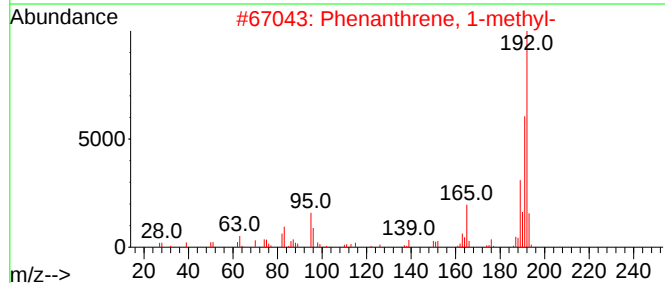
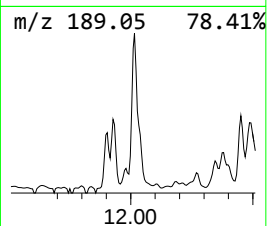
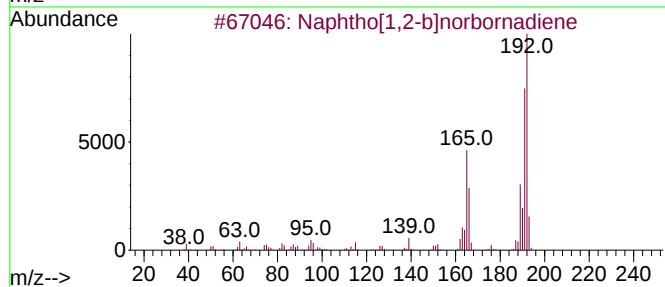
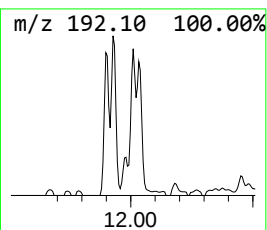
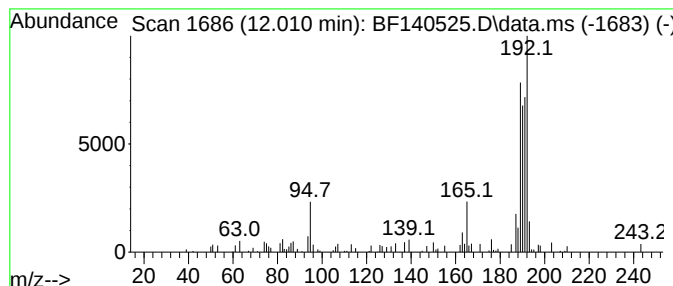
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Naphtho[1,2-b]norbornadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.84 ng	84826	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	70
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	55
3			4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	52
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	50
5			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140525.D
Acq On : 21 Nov 2024 02:35
Operator : RC/JU
Sample : P4916-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2-WC

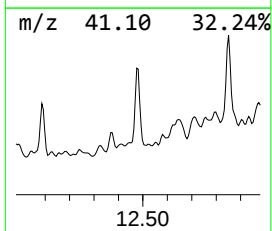
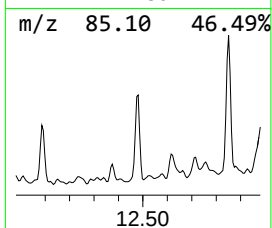
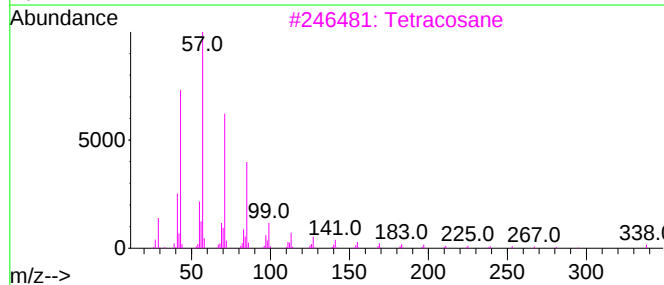
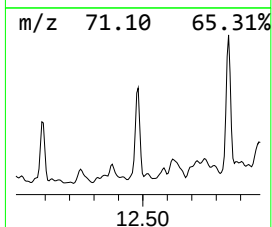
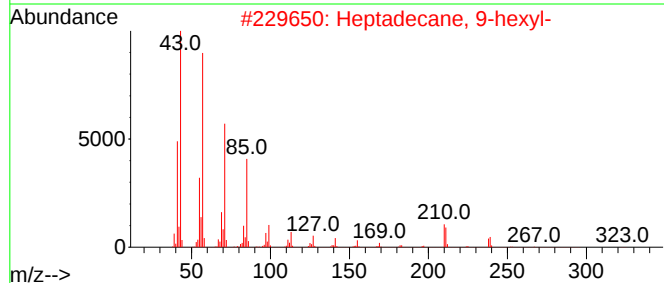
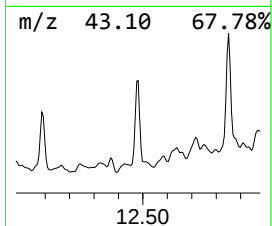
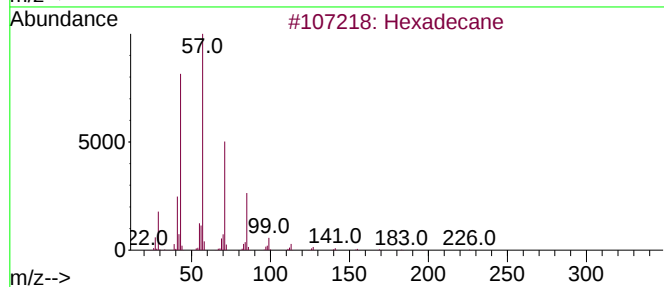
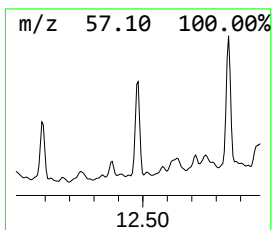
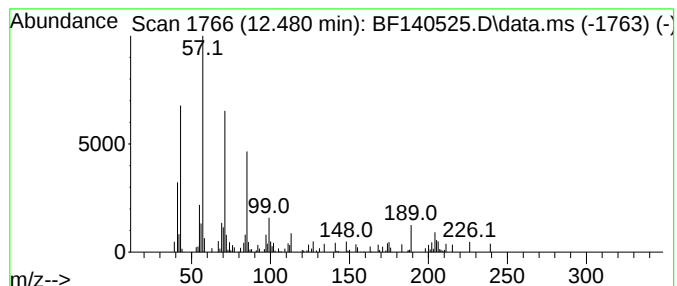
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.480	2.28 ng	68114	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	94
2			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	68
3			Tetracosane	338	C24H50	000646-31-1	62
4			Hexacosane	366	C26H54	000630-01-3	62
5			Heneicosane	296	C21H44	000629-94-7	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140525.D
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Operator : RC/JU
Sample : P4916-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

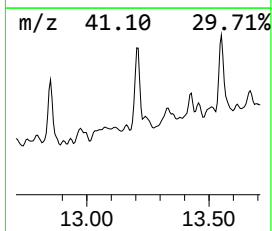
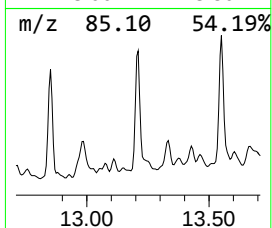
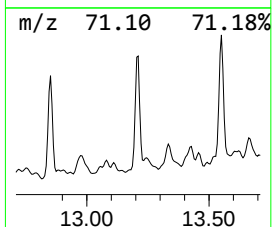
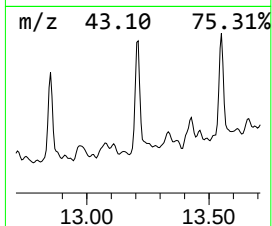
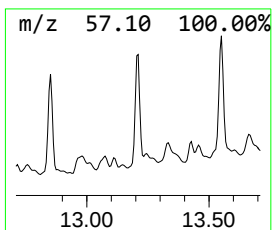
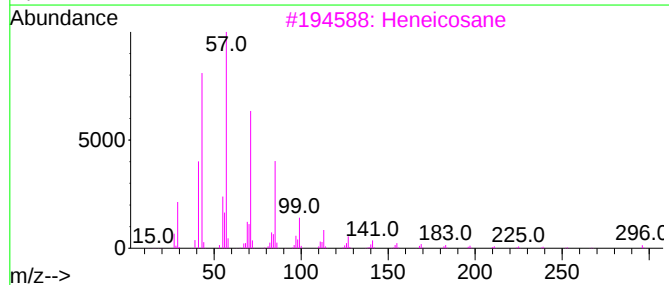
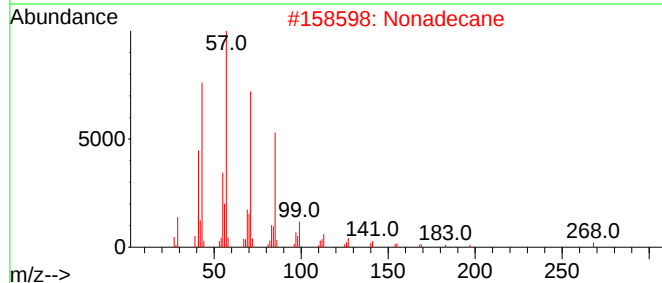
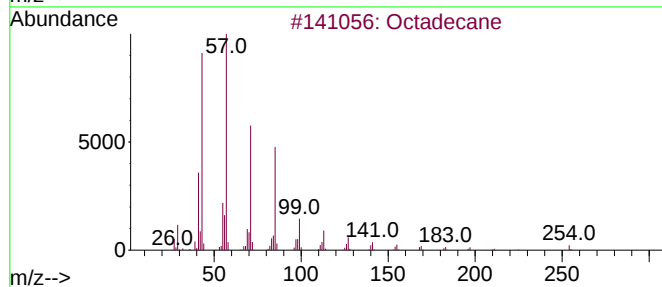
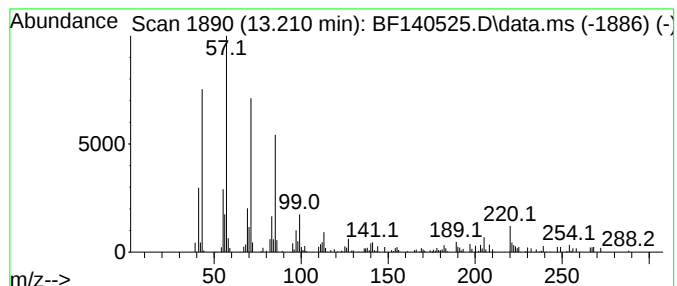
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ClientSampleId :
TP-2-WC

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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 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.210	3.04 ng	75577	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	97
2	Nonadecane	268	C19H40	000629-92-5	91
3	Heneicosane	296	C21H44	000629-94-7	83
4	Hexacosane	366	C26H54	000630-01-3	83
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140525.D
Acq On : 21 Nov 2024 02:35
Operator : RC/JU
Sample : P4916-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2-WC

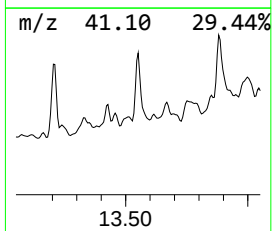
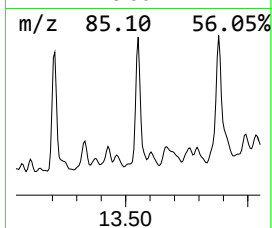
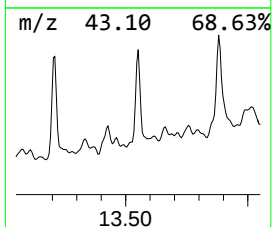
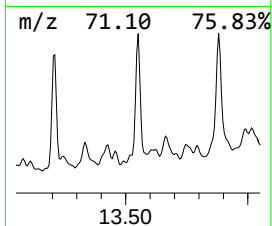
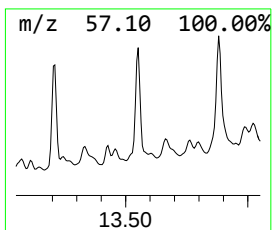
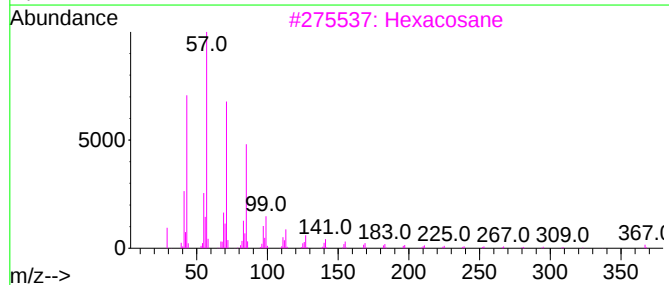
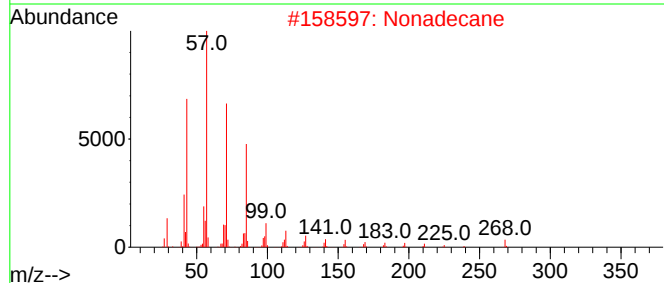
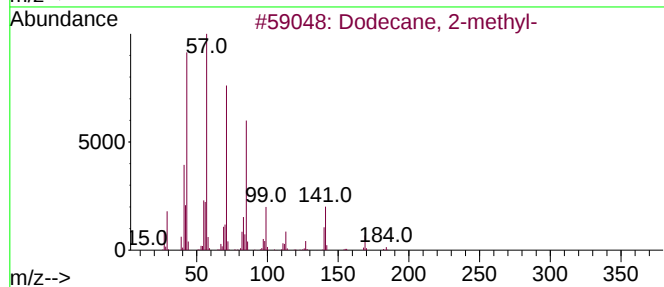
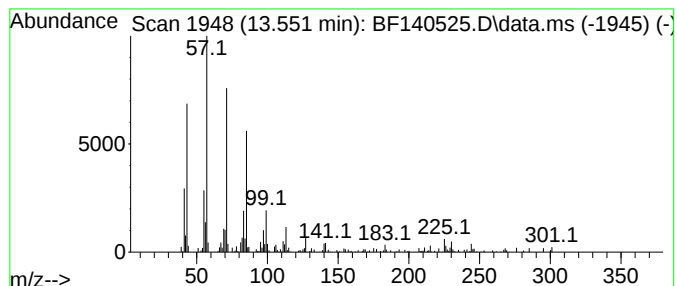
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.551	2.37 ng	59051	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2			Nonadecane	268	C19H40	000629-92-5	89
3			Hexacosane	366	C26H54	000630-01-3	87
4			Heneicosane	296	C21H44	000629-94-7	83
5			Triacontane	422	C30H62	000638-68-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140525.D
Acq On : 21 Nov 2024 02:35
Operator : RC/JU
Sample : P4916-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2-WC

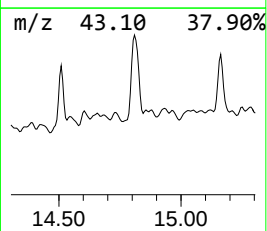
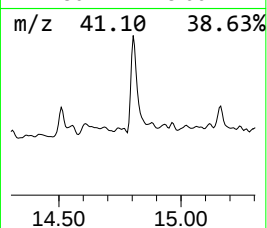
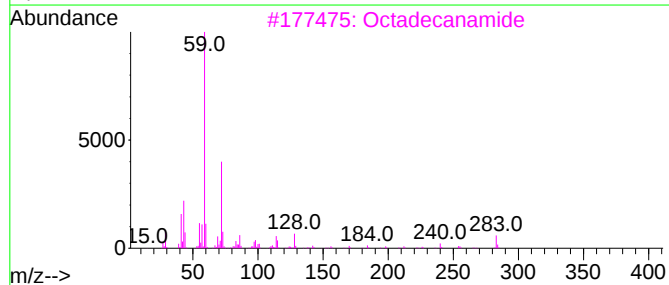
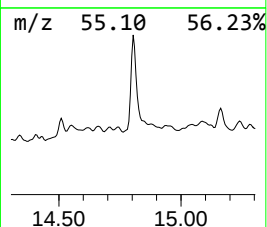
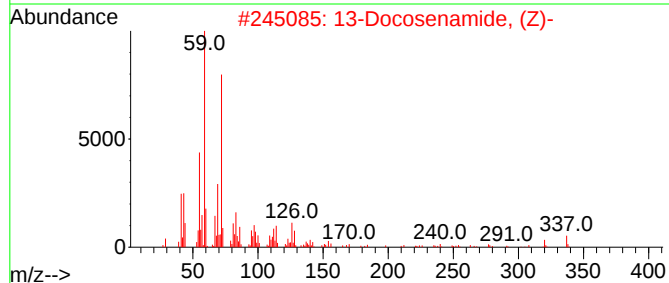
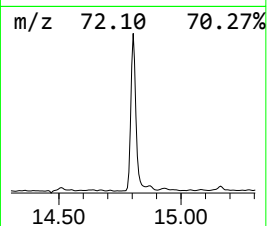
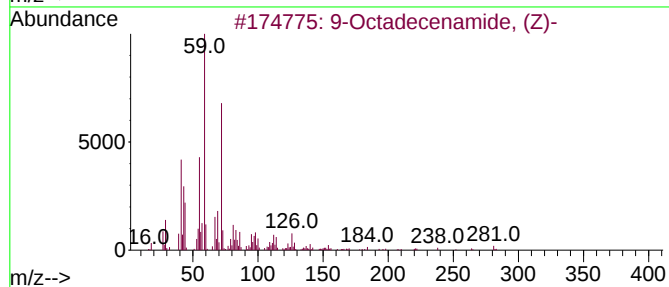
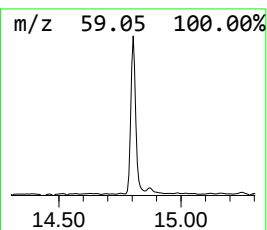
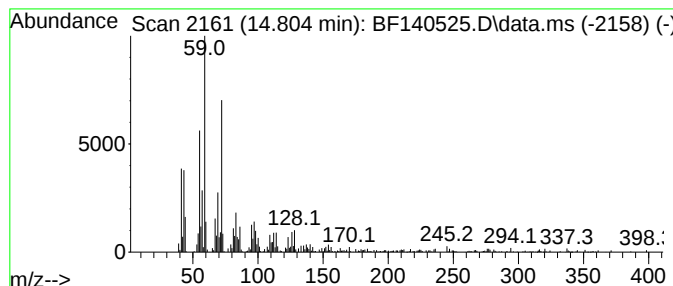
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	13.51 ng	225240	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
3			Octadecanamide	283	C18H37NO	000124-26-5	64
4			2,11-Dimethyl-2,11-dodecanediol	230	C14H30O2	022092-59-7	38
5			Hexadecanamide	255	C16H33NO	000629-54-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112024\
Data File : BF140525.D
Acq On : 21 Nov 2024 02:35
Operator : RC/JU
Sample : P4916-05
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2-WC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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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unknown9.998	9.998	10.2	ng	230271	3	9.910	453242	20.0
Benzophenone	10.622	9.4	ng	212133	3	9.910	453242	20.0
n-Hexadecanoic ...	11.922	6.2	ng	184471	4	11.398	596433	20.0
Naphtho[1,2-b]n...	12.010	2.8	ng	84826	4	11.398	596433	20.0
Hexadecane	12.480	2.3	ng	68114	4	11.398	596433	20.0
Octadecane	13.210	3.0	ng	75577	5	14.045	497663	20.0
Dodecane, 2-met...	13.551	2.4	ng	59051	5	14.045	497663	20.0
9-Octadecenamid...	14.804	13.5	ng	225240	6	15.545	333550	20.0