

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
 Data File : BF137050.D
 Acq On : 12 Jan 2024 15:59
 Operator : CG\JU
 Sample : P1104-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137050.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	19	rBV	11673	16022	1.28%	0.174%
2	5.022	495	499	506	rBV	66539	80915	6.46%	0.881%
3	5.434	565	569	584	rBV	1039923	1077568	85.98%	11.728%
4	6.434	735	739	754	rBV	1181766	1100874	87.84%	11.981%
5	6.622	766	771	775	rBV2	8439	14530	1.16%	0.158%
6	6.781	795	798	802	rBV	408462	336486	26.85%	3.662%
7	7.345	890	894	897	rBV	801343	683944	54.57%	7.444%
8	8.057	1012	1015	1031	rBV	504434	443649	35.40%	4.828%
9	9.133	1194	1198	1202	rBV	1399653	1253281	100.00%	13.640%
10	9.251	1215	1218	1227	rVB	70690	74477	5.94%	0.811%
11	9.816	1310	1314	1323	rBV	598546	484127	38.63%	5.269%
12	10.610	1445	1449	1458	rBV	768948	743562	59.33%	8.092%
13	11.310	1564	1568	1571	rBV	569708	453689	36.20%	4.938%
14	11.704	1630	1635	1638	rVB	18073	14020	1.12%	0.153%
15	11.839	1655	1658	1667	rBV2	116057	130721	10.43%	1.423%
16	12.533	1773	1776	1778	rBV	34032	29479	2.35%	0.321%
17	12.633	1790	1793	1799	rBV2	23748	32523	2.60%	0.354%
18	12.763	1810	1815	1819	rVB2	27588	33013	2.63%	0.359%
19	12.904	1835	1839	1842	rBV	1065469	866750	69.16%	9.433%
20	13.133	1875	1878	1881	rVB	25467	19986	1.59%	0.218%
21	13.386	1915	1921	1930	rBV	162617	163123	13.02%	1.775%
22	13.474	1932	1936	1940	rBV	45336	45925	3.66%	0.500%
23	13.810	1989	1993	1996	rBV	53228	47055	3.75%	0.512%
24	13.886	2001	2006	2013	rBV10	10320	31569	2.52%	0.344%
25	13.968	2016	2020	2024	rBV	348431	320656	25.59%	3.490%
26	14.074	2030	2038	2041	rVB8	7411	14468	1.15%	0.157%
27	14.127	2043	2047	2051	rBV	64704	56458	4.50%	0.614%
28	14.433	2096	2099	2102	rBV	57376	50088	4.00%	0.545%
29	14.739	2148	2151	2156	rVB	41740	42731	3.41%	0.465%
30	14.815	2161	2164	2168	rVB3	13897	15080	1.20%	0.164%
31	15.027	2196	2200	2202	rBV2	15278	21172	1.69%	0.230%
32	15.086	2207	2210	2213	rVB	23263	25061	2.00%	0.273%
33	15.333	2248	2252	2256	rBV2	15174	17874	1.43%	0.195%
34	15.398	2259	2263	2267	rVV	15423	20446	1.63%	0.223%
35	15.457	2268	2273	2282	rVV	288549	393022	31.36%	4.277%
36	16.333	2418	2422	2429	rVB9	8102	19192	1.53%	0.209%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.451	2607	2612	2614	rBV5	8583	14835	1.18%	0.161%
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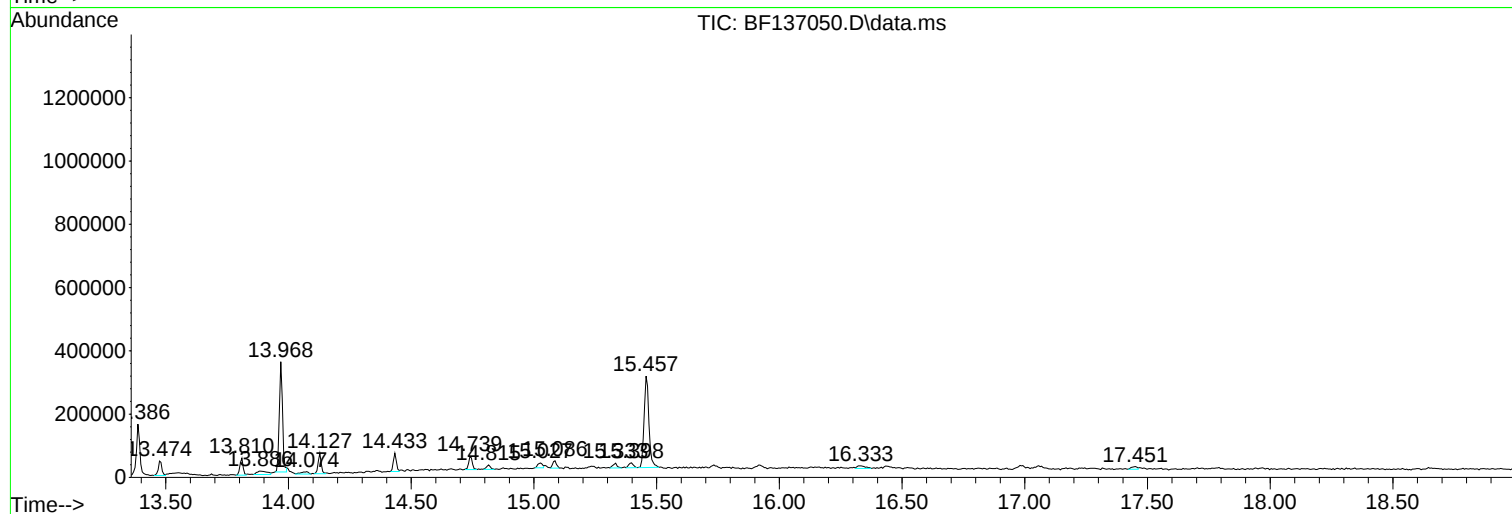
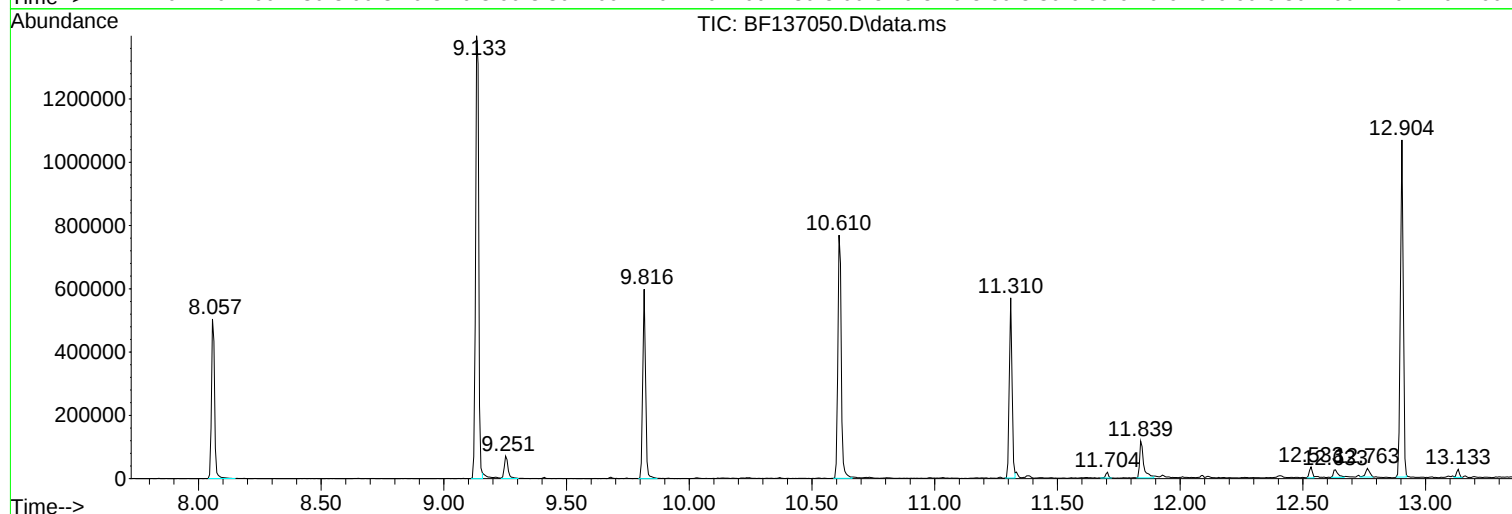
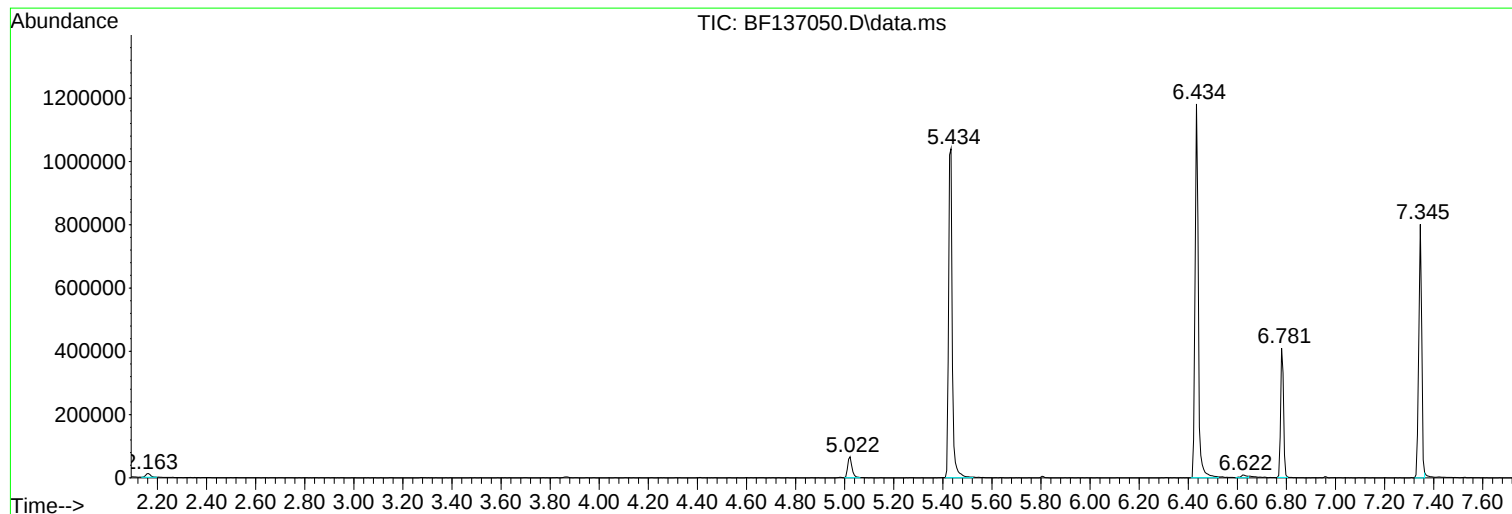
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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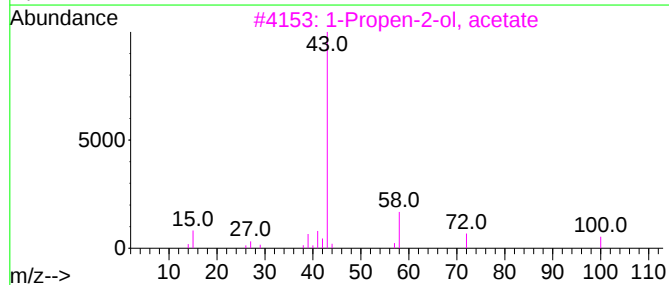
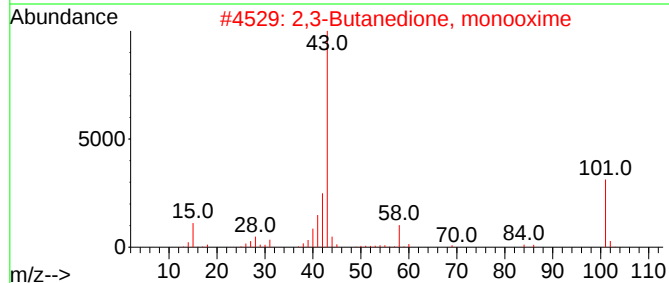
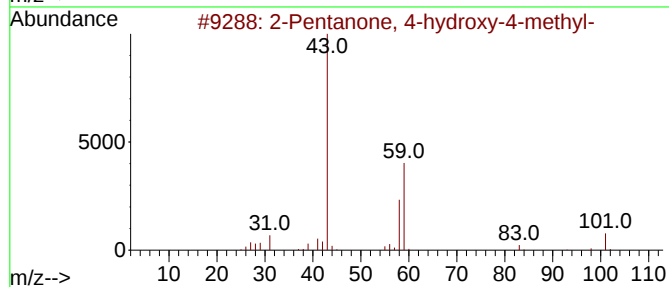
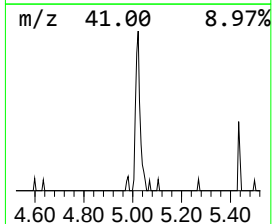
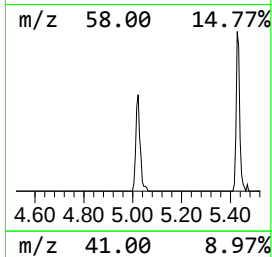
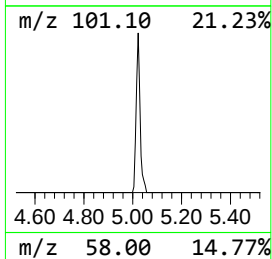
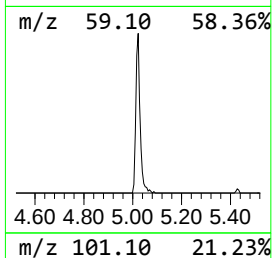
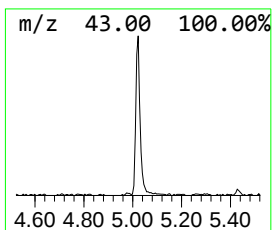
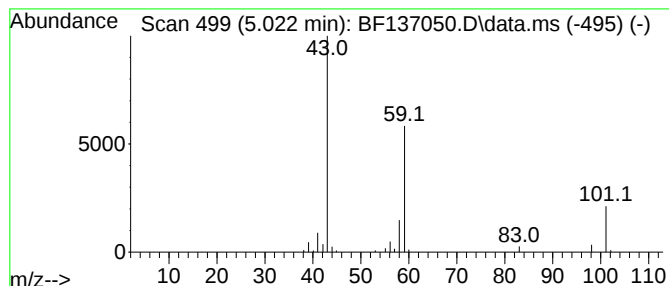
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.022	4.81 ng	80915	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9		



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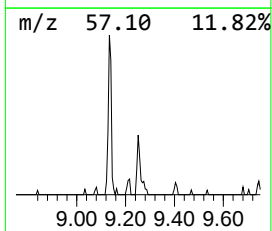
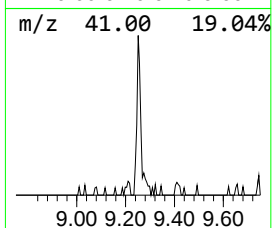
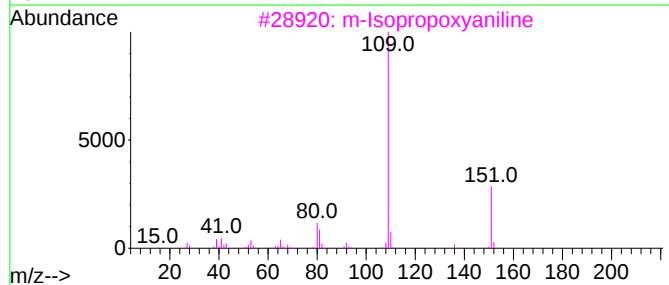
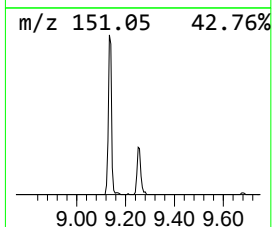
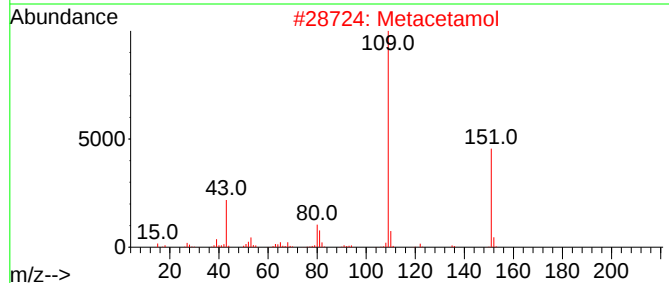
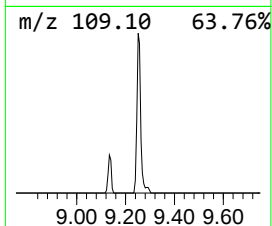
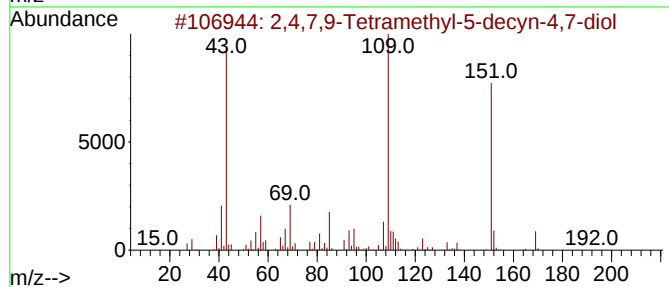
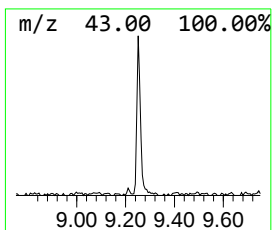
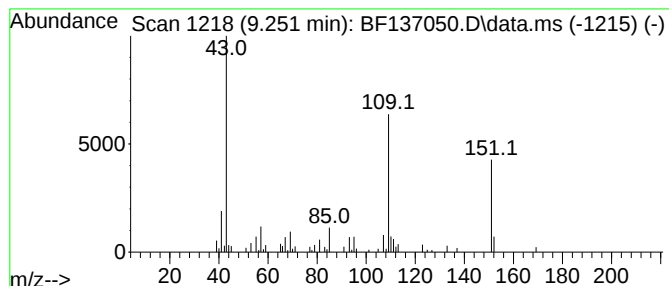
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.251	3.08 ng	74477	Acenaphthene-d10	9.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Metacetamol	151	C8H9NO2	000621-42-1	53	
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53	
4	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	42	
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	35	



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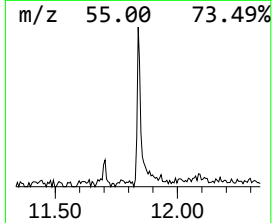
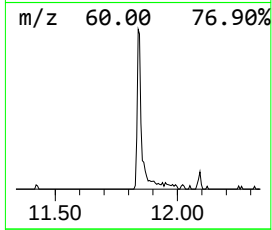
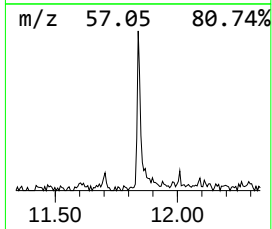
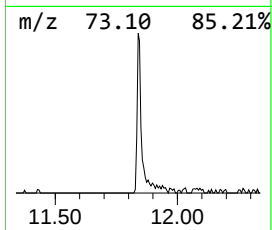
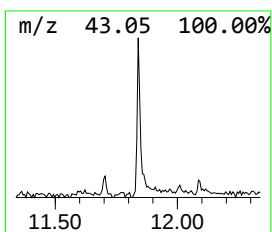
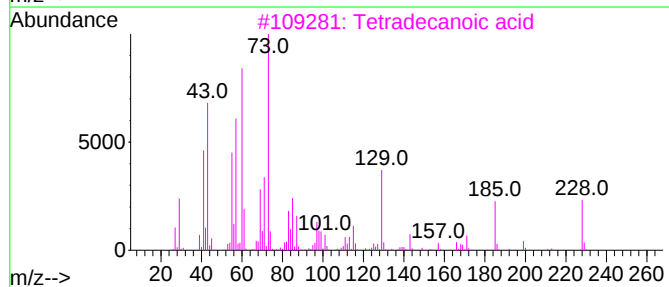
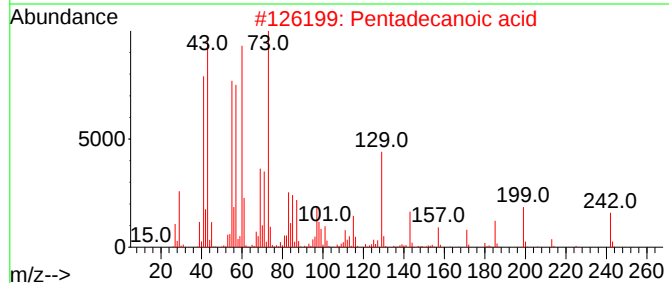
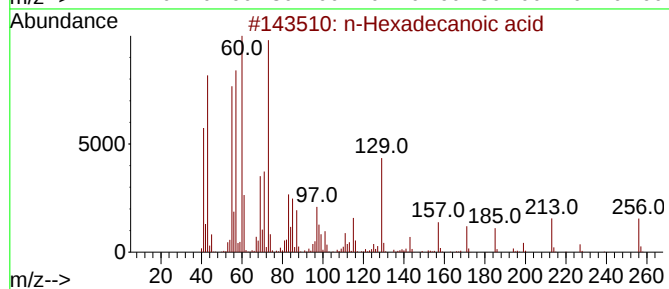
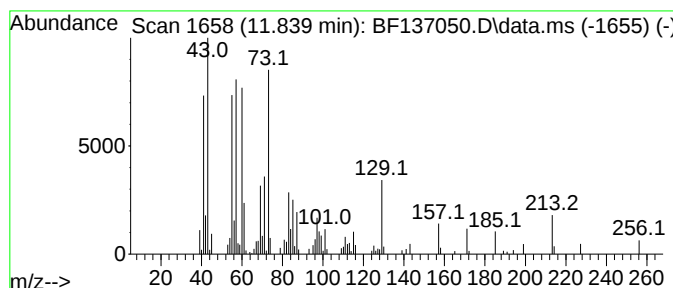
Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.839	5.76 ng	130721	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	83
4	Tridecanoic acid		214	C13H26O2	000638-53-9	74
5	n-Decanoic acid		172	C10H20O2	000334-48-5	62



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ALS Vial : 8 Sample Multiplier: 1

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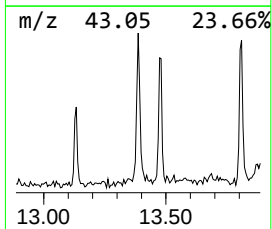
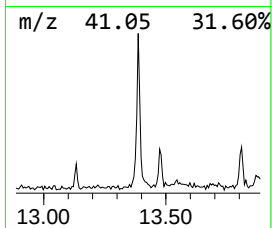
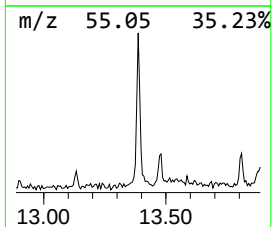
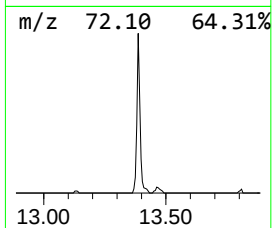
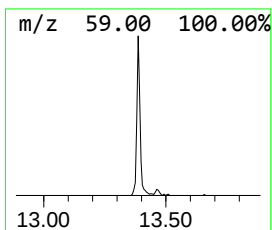
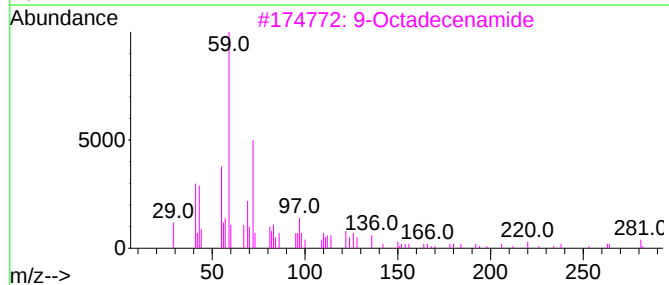
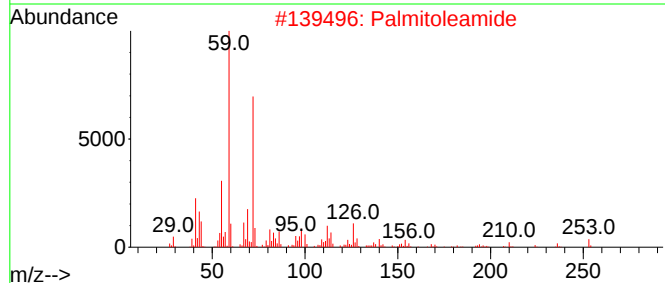
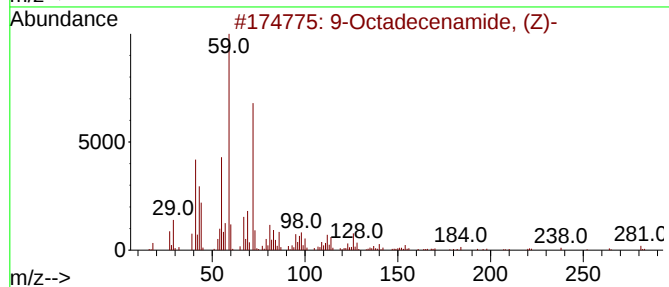
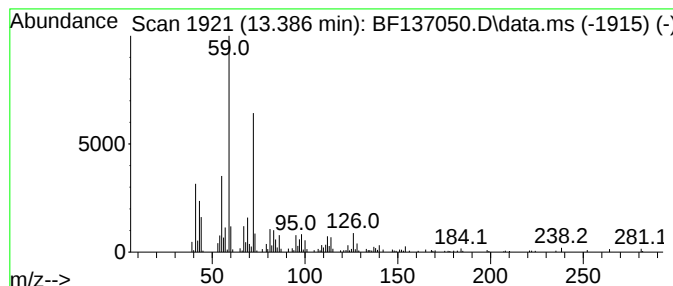
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.386	10.17 ng	163123	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2			Palmitoleamide	253	C16H31NO	106010-22-4	87
3			9-Octadecenamide	281	C18H35NO	003322-62-1	74
4			Tetradecanamide	227	C14H29NO	000638-58-4	72
5			Dodecanamide	199	C12H25NO	001120-16-7	64



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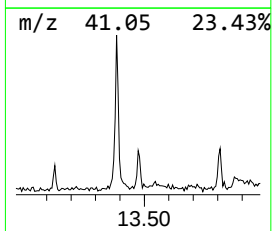
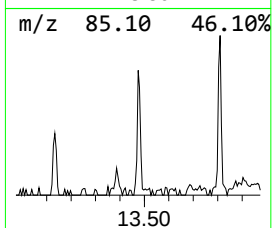
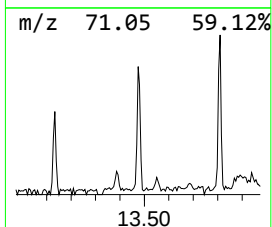
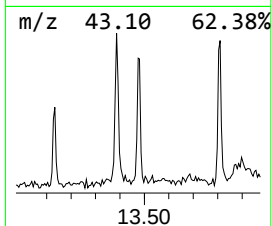
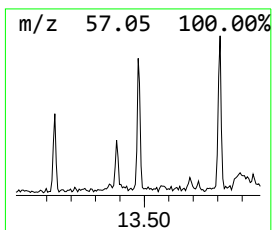
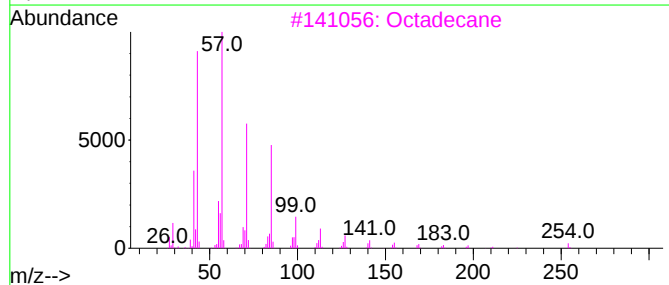
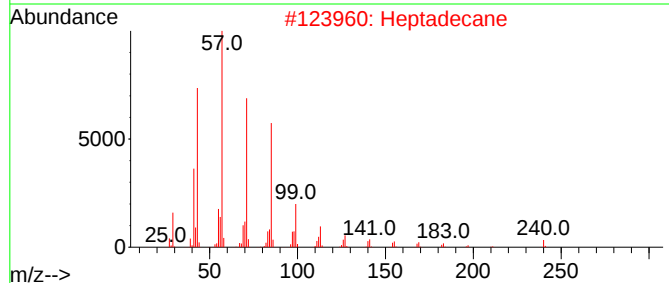
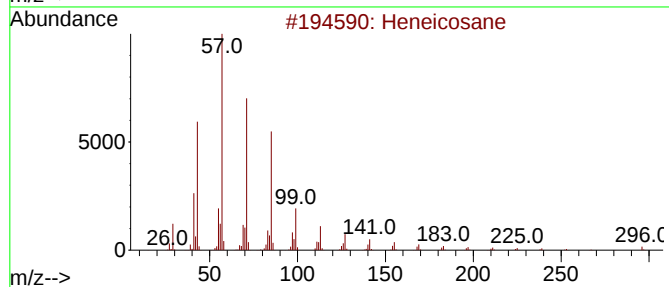
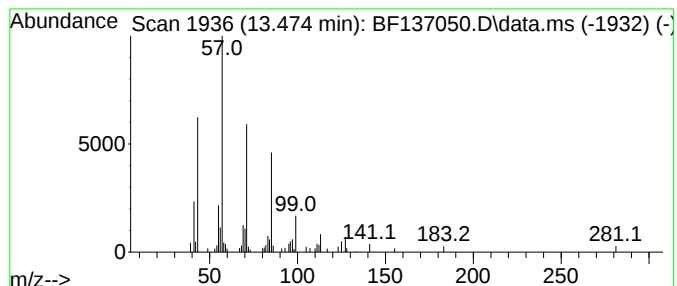
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	2.86 ng	45925	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane	240	C17H36	000629-78-7	87
3			Octadecane	254	C18H38	000593-45-3	86
4			Nonadecane	268	C19H40	000629-92-5	86
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137050.D
Acq On : 12 Jan 2024 15:59
Operator : CG\JU
Sample : P1104-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-2

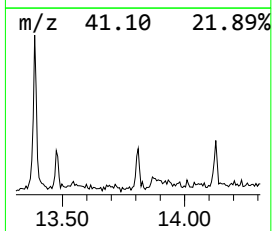
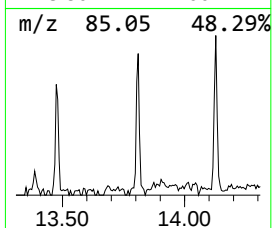
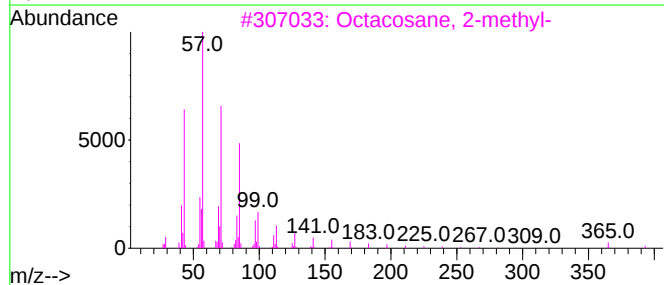
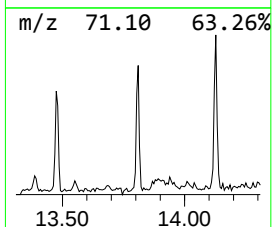
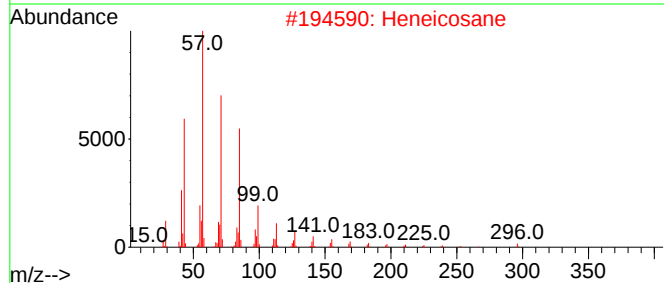
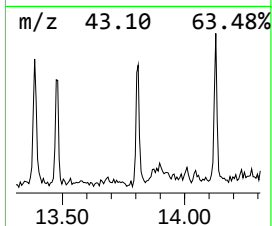
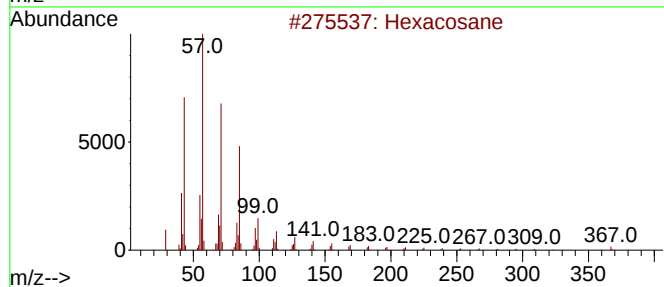
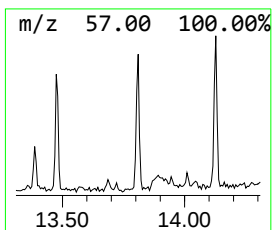
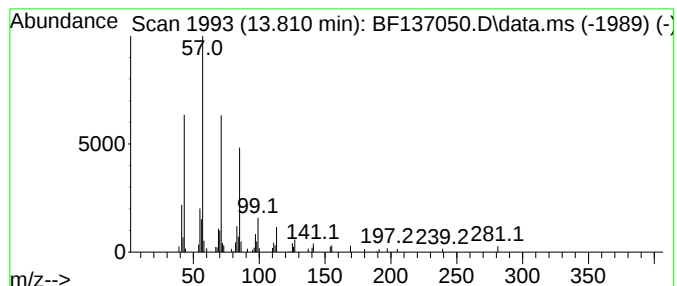
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	2.93 ng	47055	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
5			Nonadecane	268	C19H40	000629-92-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137050.D
Acq On : 12 Jan 2024 15:59
Operator : CG\JU
Sample : P1104-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

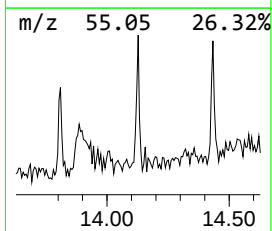
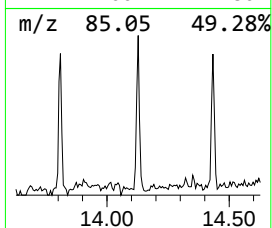
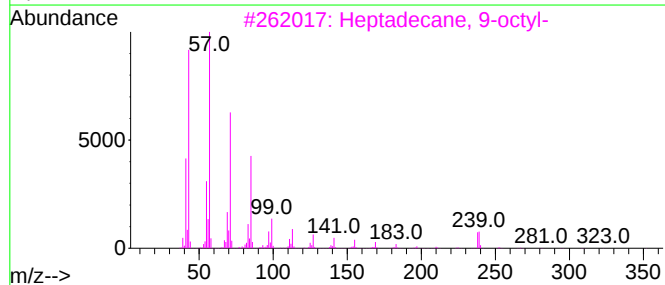
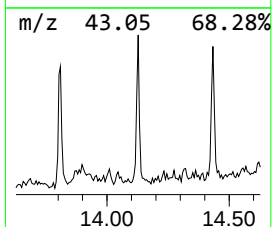
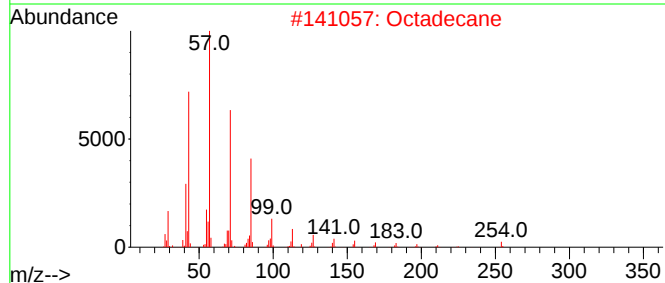
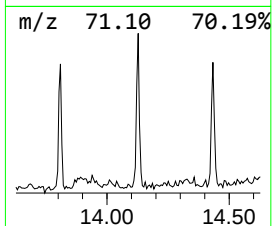
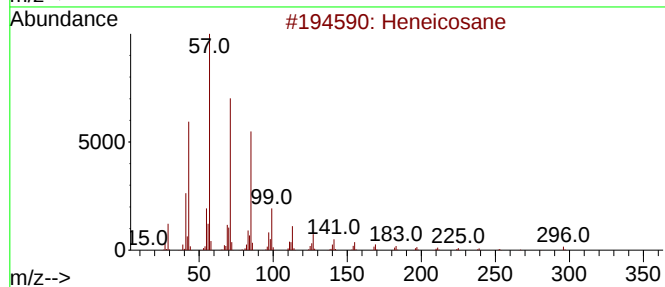
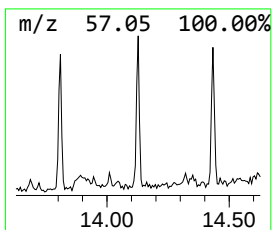
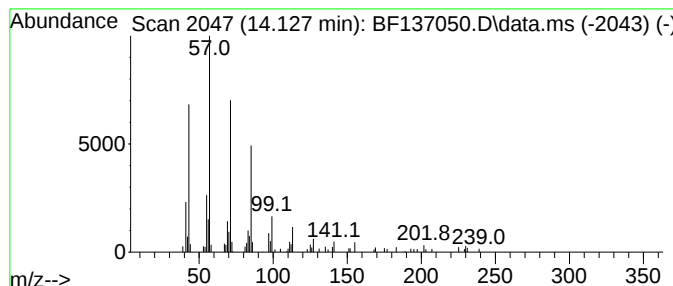
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.127	3.52 ng	56458	Chrysene-d12	13.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octadecane	254	C18H38	000593-45-3	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Docosane	310	C22H46	000629-97-0	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137050.D
Acq On : 12 Jan 2024 15:59
Operator : CG\JU
Sample : P1104-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

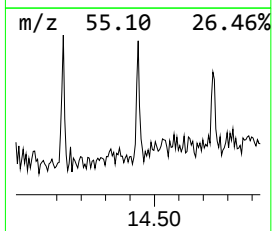
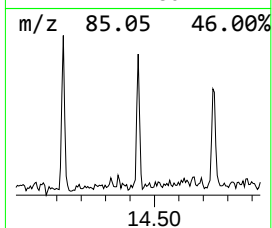
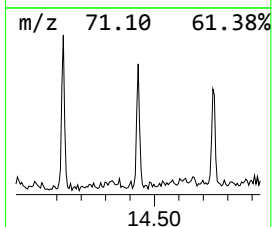
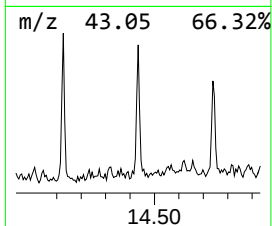
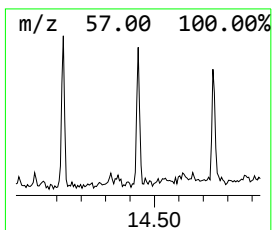
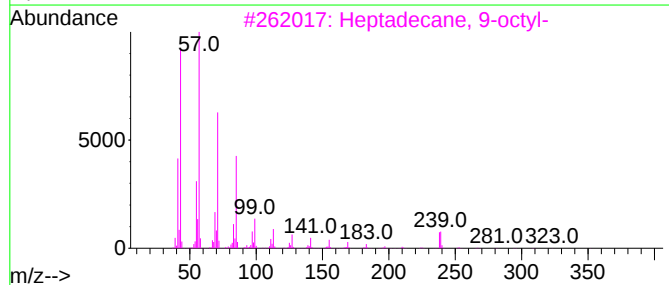
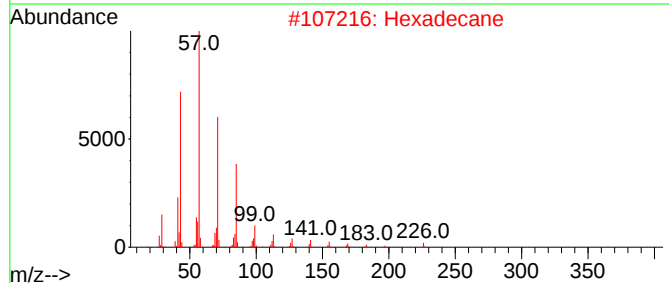
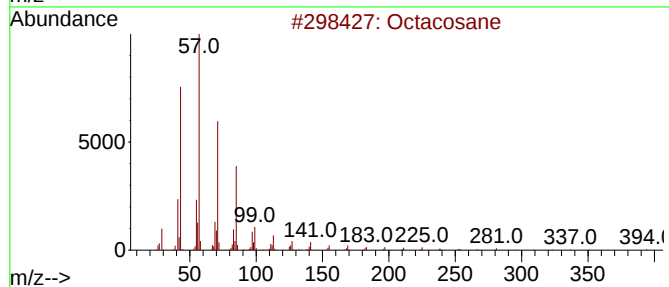
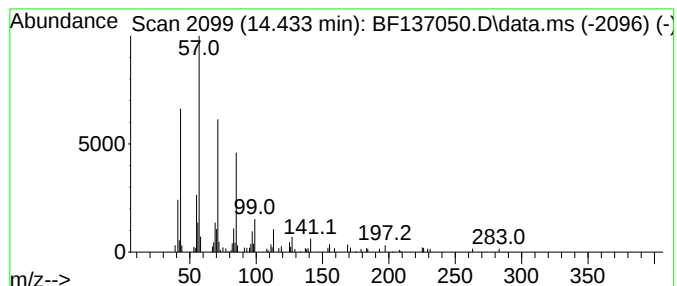
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.433	3.12 ng	50088	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Hexadecane	226	C16H34	000544-76-3	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137050.D
Acq On : 12 Jan 2024 15:59
Operator : CG\JU
Sample : P1104-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

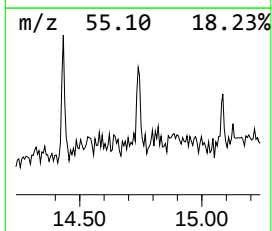
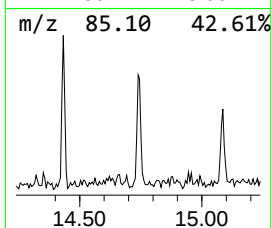
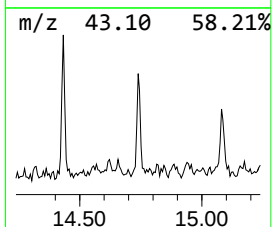
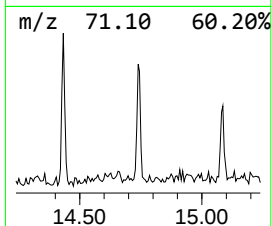
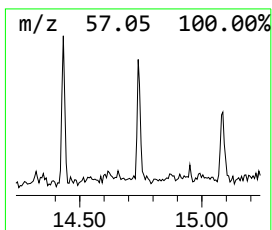
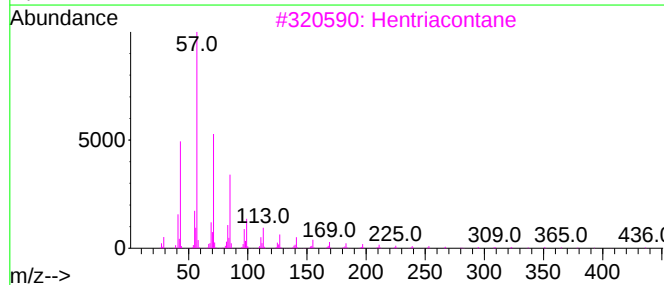
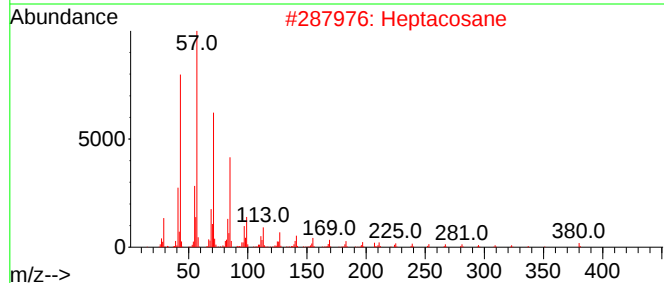
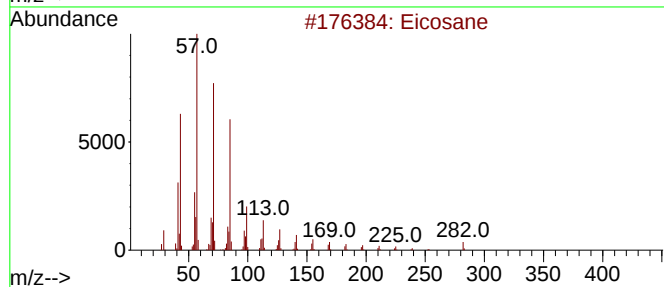
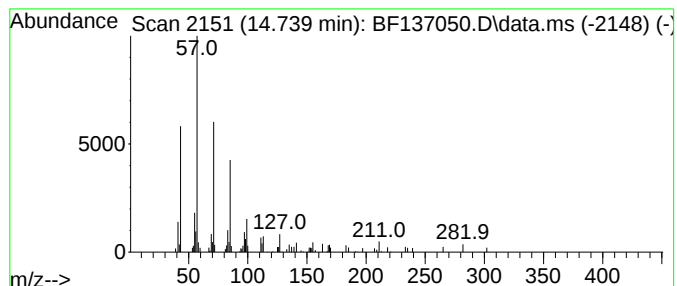
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	2.17 ng	42731	Perylene-d12	15.457

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	96
2		Heptacosane	380	C27H56	000593-49-7	83
3		Hentriacontane	437	C31H64	000630-04-6	83
4		Docosane	310	C22H46	000629-97-0	83
5		Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137050.D
Acq On : 12 Jan 2024 15:59
Operator : CG\JU
Sample : P1104-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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2,4,7,9-Tetrame...	9.251	3.1	ng	74477	3	9.816	484127	20.0
n-Hexadecanoic ...	11.839	5.8	ng	130721	4	11.310	453689	20.0
9-Octadecenamid...	13.386	10.2	ng	163123	5	13.969	320656	20.0
Heneicosane	13.474	2.9	ng	45925	5	13.969	320656	20.0
Hexacosane	13.810	2.9	ng	47055	5	13.969	320656	20.0
Octadecane	14.127	3.5	ng	56458	5	13.969	320656	20.0
Octacosane	14.433	3.1	ng	50088	5	13.969	320656	20.0
Eicosane	14.739	2.2	ng	42731	6	15.457	393022	20.0