

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080823\
 Data File : BF134667.D
 Acq On : 08 Aug 2023 12:40
 Operator : CG\JU
 Sample : 03913-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11933

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.158	7	12	20	rVB3	51226	81314	2.67%	0.304%
2	5.022	495	499	506	rVB	212265	233562	7.66%	0.873%
3	5.422	563	567	571	rBV	2969770	3002880	98.45%	11.225%
4	6.428	733	738	741	rBV	3055296	2963965	97.17%	11.079%
5	6.622	769	771	776	rBV3	39064	42373	1.39%	0.158%
6	6.798	797	801	804	rBV	1272346	1077688	35.33%	4.028%
7	7.357	891	896	899	rBV	2168892	1852751	60.74%	6.926%
8	8.075	1013	1018	1021	rBV	1655789	1358281	44.53%	5.077%
9	9.151	1197	1201	1204	rBV	3901277	3050255	100.00%	11.402%
10	9.234	1210	1215	1218	rBV	75368	75347	2.47%	0.282%
11	9.686	1289	1292	1296	rBV	34912	42252	1.39%	0.158%
12	9.769	1303	1306	1310	rVB	62124	55741	1.83%	0.208%
13	9.828	1310	1316	1320	rBV	1574974	1278238	41.91%	4.778%
14	10.269	1388	1391	1393	rVB	66324	50842	1.67%	0.190%
15	10.616	1446	1450	1453	rBV	1772143	1453305	47.65%	5.433%
16	10.745	1469	1472	1477	rBV2	102691	143097	4.69%	0.535%
17	11.192	1545	1548	1550	rBV	84193	64010	2.10%	0.239%
18	11.222	1550	1553	1559	rVB2	55312	74673	2.45%	0.279%
19	11.316	1566	1569	1571	rBV	1341592	1080162	35.41%	4.038%
20	11.339	1571	1573	1577	rVV	419263	314271	10.30%	1.175%
21	11.392	1579	1582	1585	rVB	81859	77906	2.55%	0.291%
22	11.622	1618	1621	1623	rBV2	81348	64878	2.13%	0.243%
23	11.722	1636	1638	1643	rVB4	29657	39527	1.30%	0.148%
24	11.822	1652	1655	1657	rBV	51796	49219	1.61%	0.184%
25	11.857	1657	1661	1665	rBV2	445740	443731	14.55%	1.659%
26	11.928	1670	1673	1676	rBV2	88798	95355	3.13%	0.356%
27	12.028	1688	1690	1693	rBV	84936	74458	2.44%	0.278%
28	12.139	1707	1709	1713	rVB2	65395	67287	2.21%	0.252%
29	12.375	1746	1749	1751	rBV	73988	73228	2.40%	0.274%
30	12.404	1751	1754	1756	rBV3	79686	110363	3.62%	0.413%
31	12.533	1772	1776	1779	rBV	828035	685650	22.48%	2.563%
32	12.645	1792	1795	1800	rBV3	136517	163580	5.36%	0.611%
33	12.763	1810	1815	1818	rBV	679649	674423	22.11%	2.521%
34	12.798	1818	1821	1823	rVV2	67124	63029	2.07%	0.236%
35	12.910	1837	1840	1844	rBV	2828090	2722422	89.25%	10.177%
36	13.092	1869	1871	1875	rVB	141335	110585	3.63%	0.413%

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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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.157	1879	1882	1885	rVV2	157904	128838	4.22%	0.482%
38	13.192	1886	1888	1891	rBV	80913	94882	3.11%	0.355%
39	13.498	1938	1940	1942	rBV	101106	86494	2.84%	0.323%
40	13.827	1993	1996	2003	rVB2	288661	397552	13.03%	1.486%
41	13.963	2015	2019	2022	rBV2	1176044	1426570	46.77%	5.333%
42	13.992	2022	2024	2026	rVB	314664	235159	7.71%	0.879%
43	15.439	2267	2270	2273	rVB	546206	571855	18.75%	2.138%

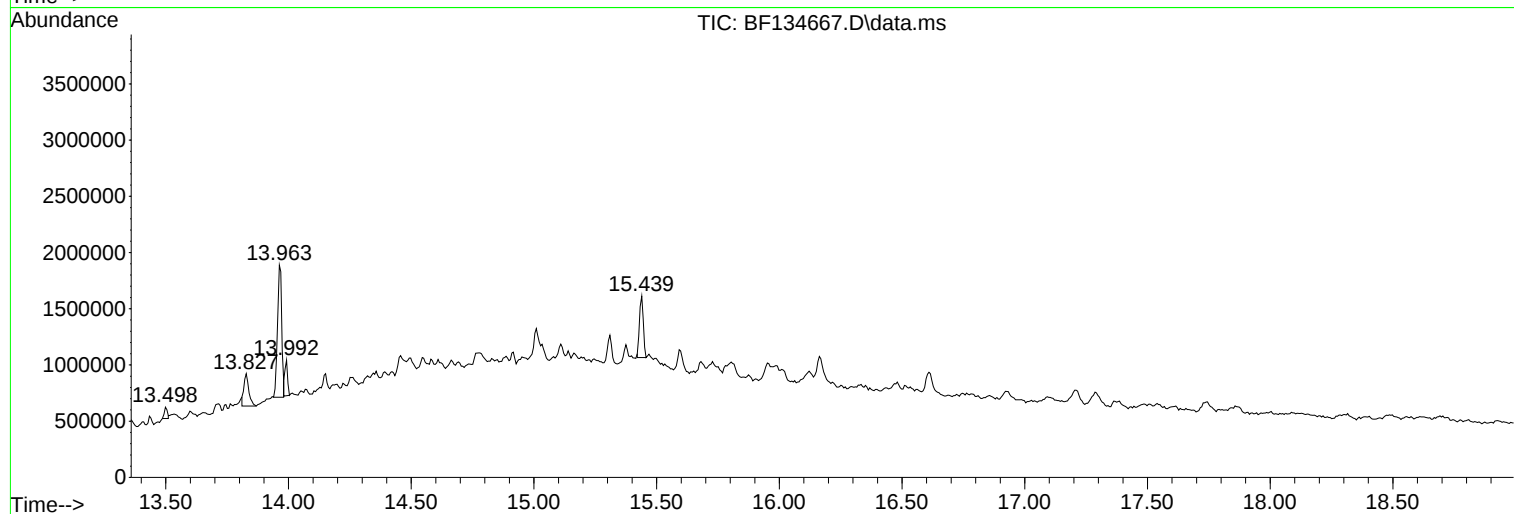
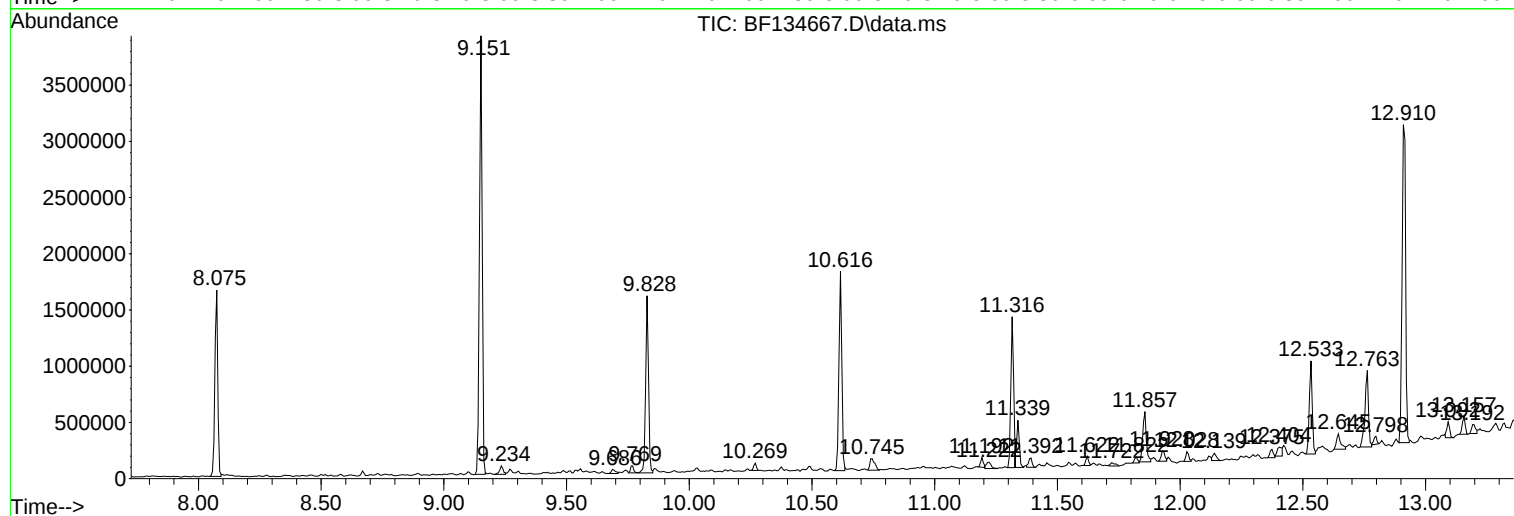
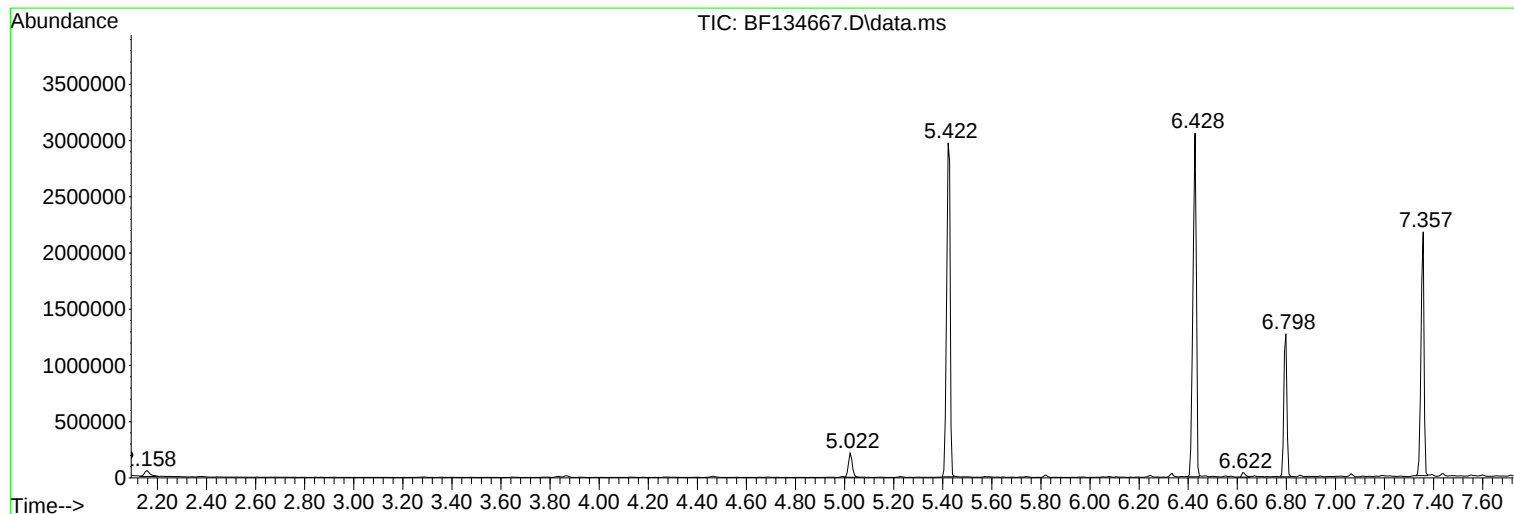
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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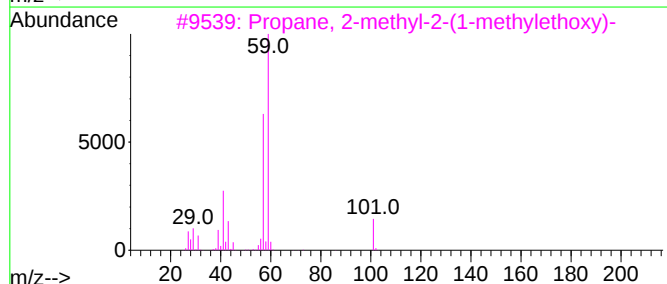
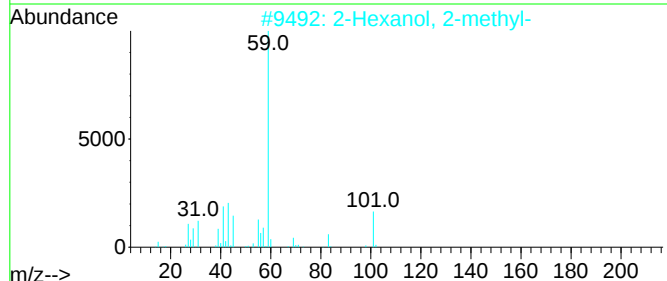
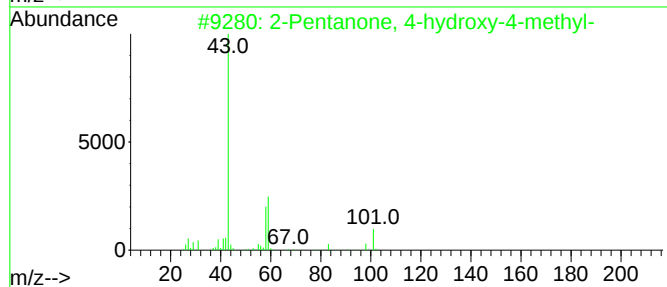
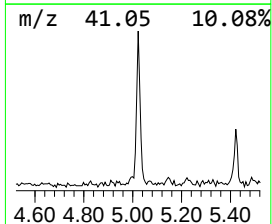
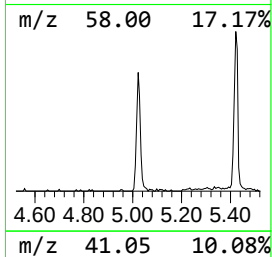
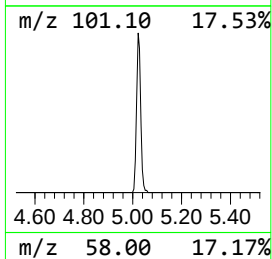
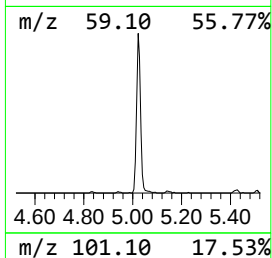
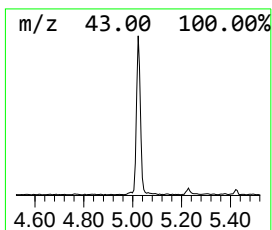
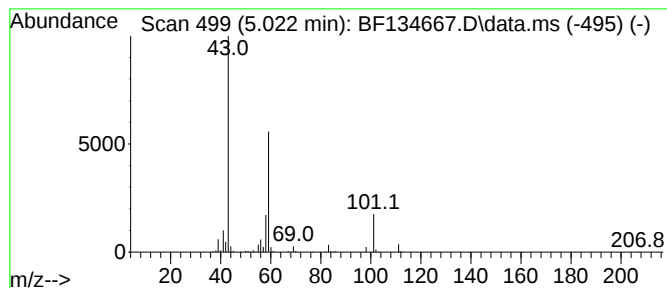
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	4.33 ng	233562	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25		
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	22		



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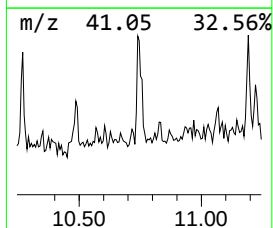
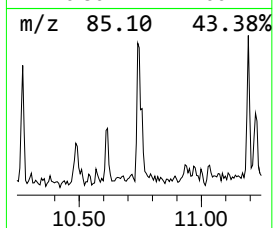
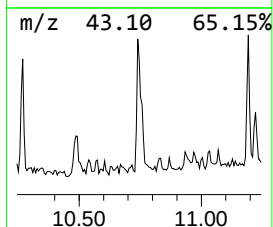
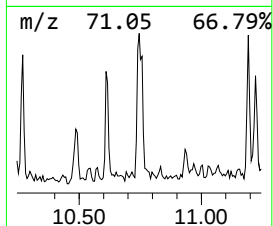
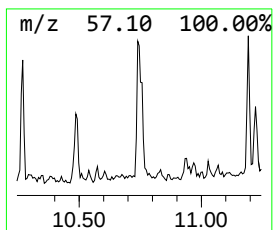
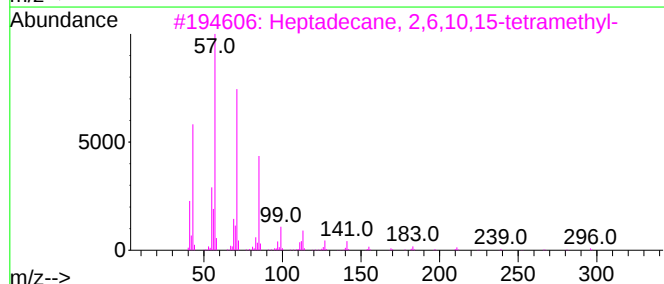
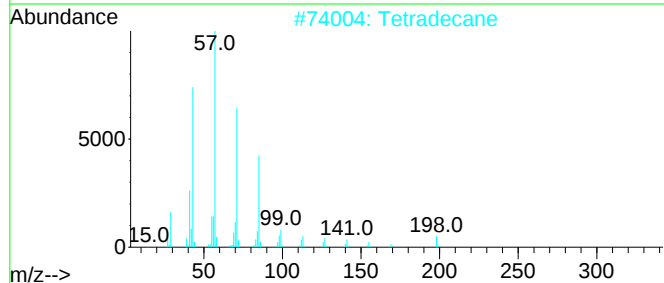
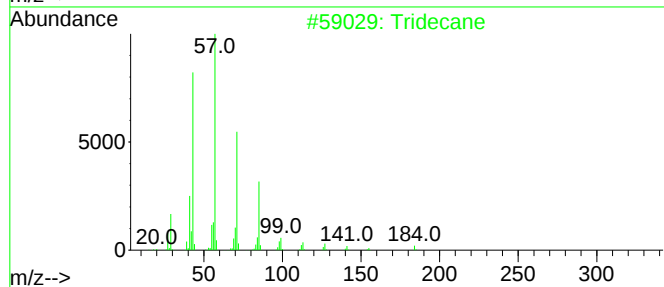
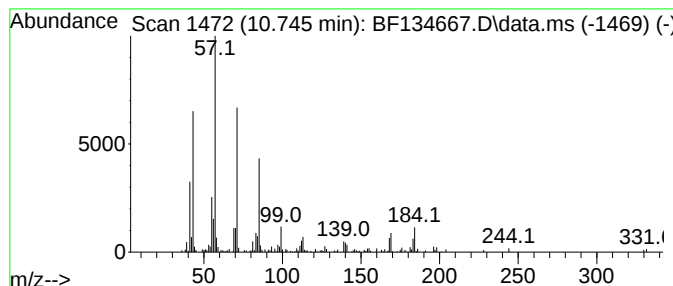
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	2.65 ng	143097	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	90
2			Tetradecane	198	C14H30	000629-59-4	87
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
4			Eicosane	282	C20H42	000112-95-8	52
5			Heptacosane	380	C27H56	000593-49-7	52



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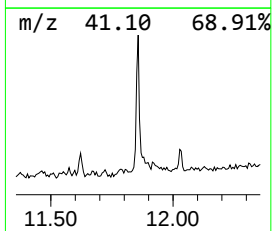
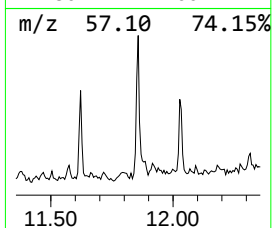
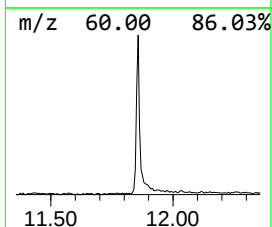
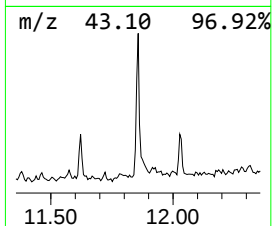
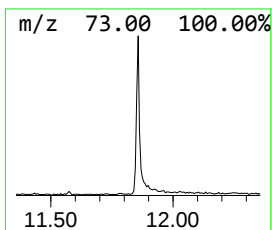
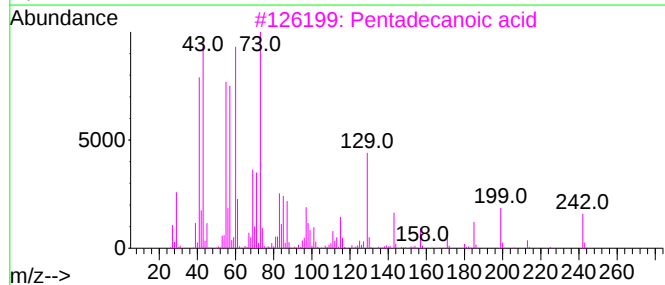
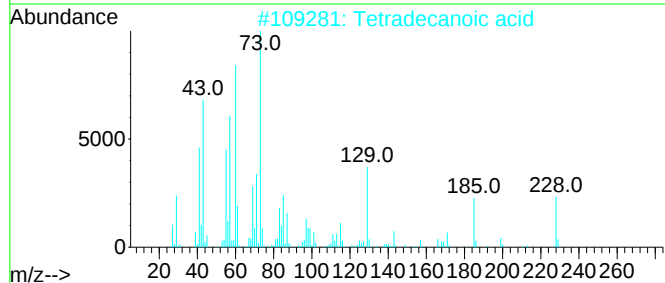
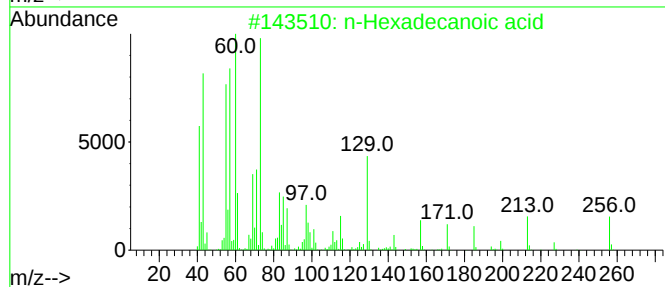
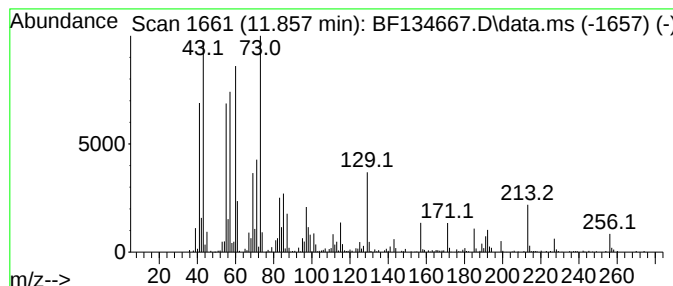
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.22 ng	443731	Phenanthrene-d10	11.316

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		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tridecanoic acid	214	C13H26O2	000638-53-9	70
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



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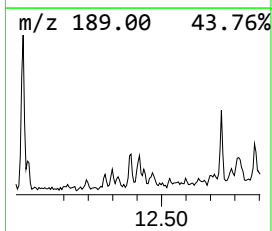
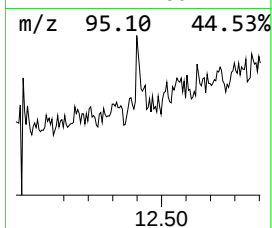
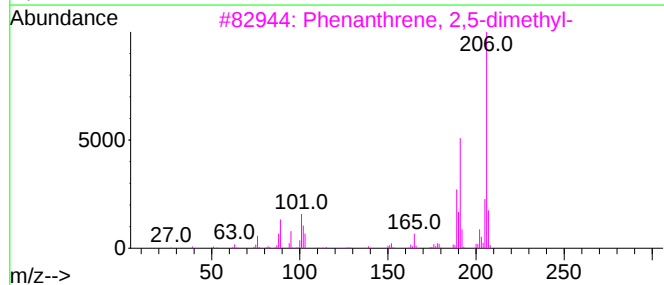
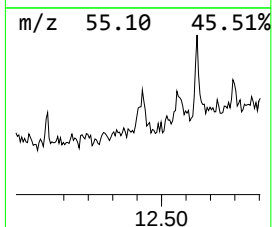
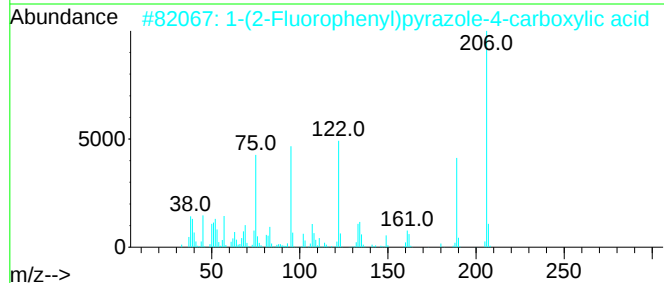
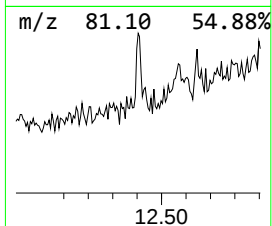
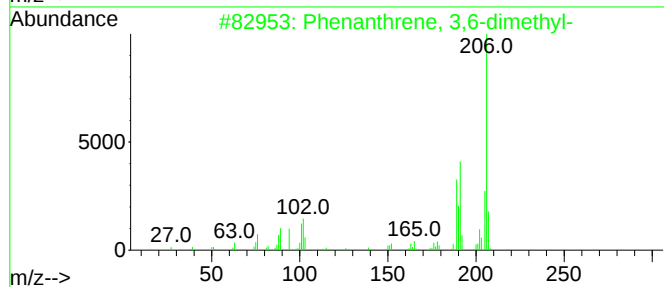
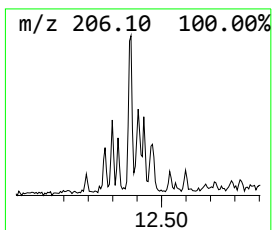
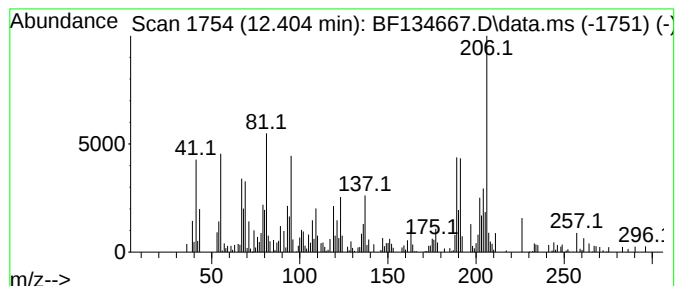
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.404	2.04 ng	110363	Phenanthrene-d10			11.316
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-		206	C16H14	001576-67-6	55
2	1-(2-Fluorophenyl)pyrazole-4-car...		206	C10H7FN2O2	1000387-97-3	45
3	Phenanthrene, 2,5-dimethyl-		206	C16H14	003674-66-6	43
4	Phenanthrene, 2,3-dimethyl-		206	C16H14	003674-65-5	41
5	9,10-Dimethylanthracene		206	C16H14	000781-43-1	38



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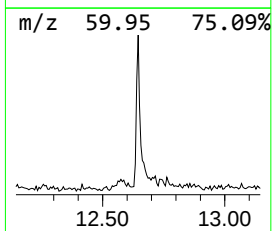
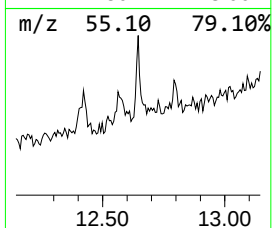
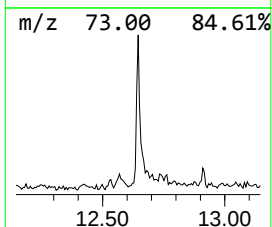
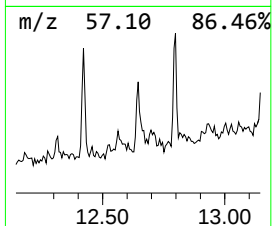
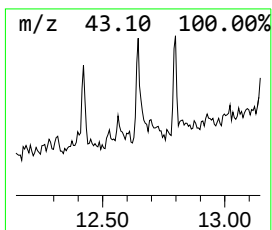
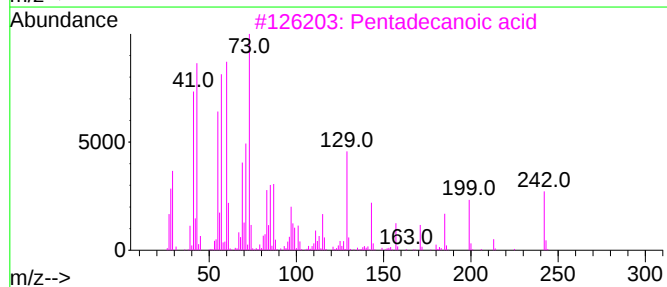
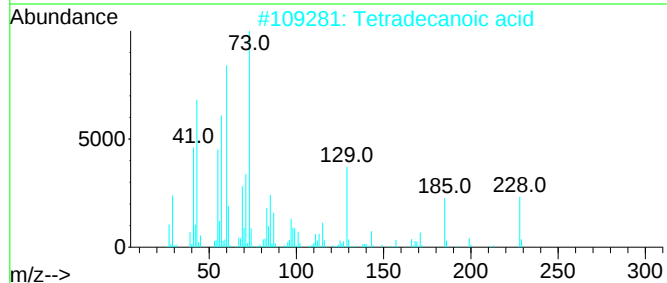
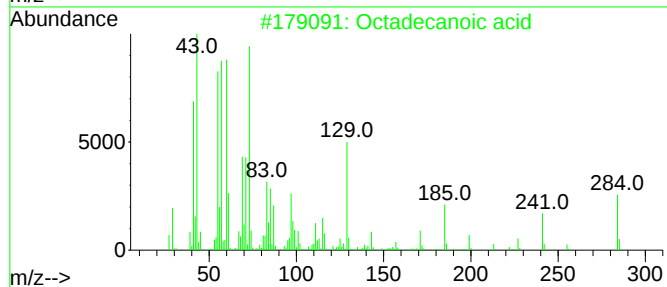
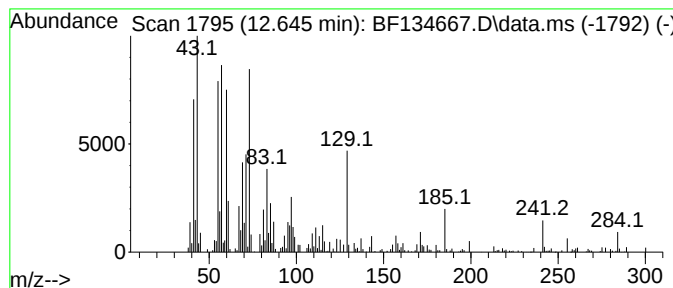
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.29 ng	163580	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			1-(Ethenesulfonyl)dodecane	260	C14H28O2S	030719-66-5	47
5			n-Decanoic acid	172	C10H20O2	000334-48-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080823\
Data File : BF134667.D
Acq On : 08 Aug 2023 12:40
Operator : CG\JU
Sample : 03913-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11933

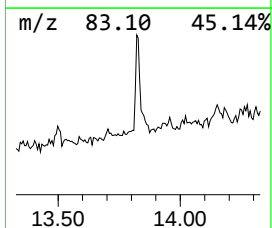
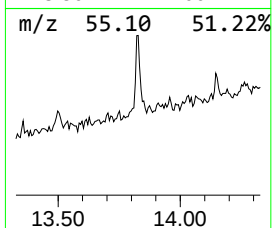
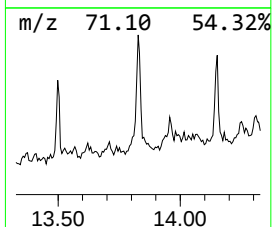
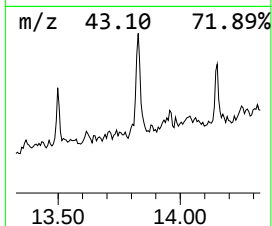
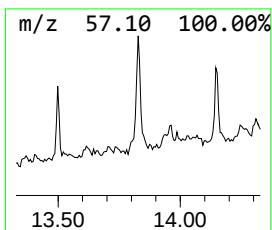
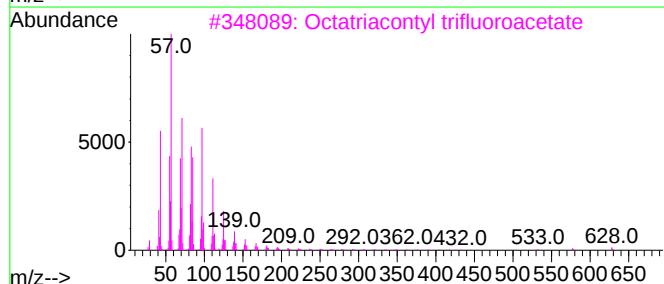
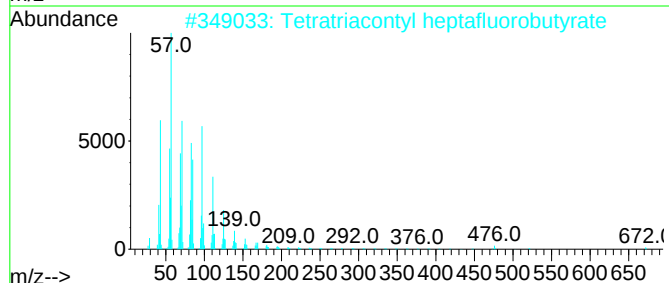
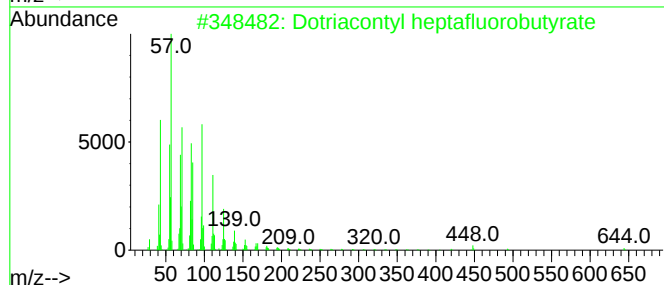
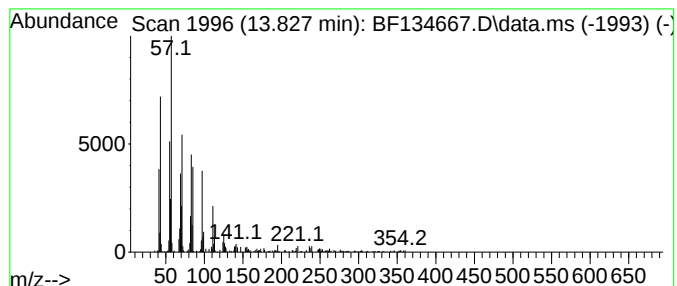
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dotriacontyl heptafluorobut... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	5.57 ng	397552	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
2			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	91
3			Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	90
4			Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	90
5			Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080823\
Data File : BF134667.D
Acq On : 08 Aug 2023 12:40
Operator : CG\JU
Sample : 03913-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11933

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	4.3	ng	233562	1	6.798	1077690	20.0
Tridecane	10.745	2.6	ng	143097	4	11.316	1080160	20.0
n-Hexadecanoic ...	11.857	8.2	ng	443731	4	11.316	1080160	20.0
Phenanthrene, 3...	12.404	2.0	ng	110363	4	11.316	1080160	20.0
Octadecanoic acid	12.645	2.3	ng	163580	5	13.969	1426570	20.0
Dotriacontyl he...	13.827	5.6	ng	397552	5	13.969	1426570	20.0