

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021325\
 Data File : BF141620.D
 Acq On : 13 Feb 2025 17:42
 Operator : RC/JU
 Sample : Q1353-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 346

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-BF020625.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141620.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	493	498	509	rVB	23132	42649	1.10%	0.157%
2	5.416	559	565	593	rBV	2205080	3131960	81.01%	11.494%
3	6.428	730	737	765	rBV	2190157	3251770	84.11%	11.933%
4	6.781	792	797	805	rBV	462184	597443	15.45%	2.193%
5	7.351	887	894	905	rBV	1458830	2132900	55.17%	7.827%
6	7.604	933	937	959	rVB	50251	90356	2.34%	0.332%
7	8.063	1010	1015	1034	rBV	577213	874063	22.61%	3.208%
8	8.781	1132	1137	1143	rBV	29760	39799	1.03%	0.146%
9	9.145	1192	1199	1209	rBV	2764585	3866208	100.00%	14.188%
10	9.816	1307	1313	1317	rBV	685155	918636	23.76%	3.371%
11	9.851	1317	1319	1328	rVB	77138	87573	2.27%	0.321%
12	10.028	1344	1349	1354	rBV	40919	56855	1.47%	0.209%
13	10.369	1402	1407	1413	rVB	54121	68788	1.78%	0.252%
14	10.533	1427	1435	1442	rVB	304457	396766	10.26%	1.456%
15	10.610	1442	1448	1464	rBV	1708110	2296596	59.40%	8.428%
16	11.304	1561	1566	1575	rBV2	674511	1311044	33.91%	4.811%
17	11.380	1575	1579	1586	rVB	34624	52972	1.37%	0.194%
18	11.839	1653	1657	1667	rVV2	129089	264419	6.84%	0.970%
19	11.922	1667	1671	1680	rVB	58887	115626	2.99%	0.424%
20	12.086	1694	1699	1704	rBV2	33111	67603	1.75%	0.248%
21	12.516	1767	1772	1778	rBV	426457	564225	14.59%	2.071%
22	12.610	1785	1788	1791	rVB2	39816	44588	1.15%	0.164%
23	12.745	1801	1811	1817	rVV	342676	642871	16.63%	2.359%
24	12.892	1828	1836	1844	rBV	2480588	3301125	85.38%	12.115%
25	12.969	1844	1849	1854	rVB2	22610	41154	1.06%	0.151%
26	13.074	1859	1867	1871	rVB2	42829	86837	2.25%	0.319%
27	13.139	1871	1878	1881	rBV2	28583	50913	1.32%	0.187%
28	13.692	1967	1972	1975	rBV2	31690	50419	1.30%	0.185%
29	13.792	1986	1989	1993	rVB	43472	53140	1.37%	0.195%
30	13.945	2007	2015	2028	rBV2	512810	1003498	25.96%	3.683%
31	14.416	2091	2095	2100	rBV3	34626	53683	1.39%	0.197%
32	14.980	2185	2191	2199	rBV	139463	305459	7.90%	1.121%
33	15.045	2199	2202	2206	rVB2	48432	63088	1.63%	0.232%
34	15.274	2236	2241	2246	rVB	77952	123702	3.20%	0.454%
35	15.333	2246	2251	2256	rVV	91979	137959	3.57%	0.506%
36	15.398	2256	2262	2274	rVB	316651	579444	14.99%	2.126%

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37	15.839	2329	2337	2345	rBV	55976	127908	3.31%	0.469%
38	16.098	2378	2381	2390	rVB7	33299	58313	1.51%	0.214%
39	16.827	2499	2505	2513	rVB2	44486	94080	2.43%	0.345%
40	16.909	2514	2519	2527	rVB2	23594	49134	1.27%	0.180%
41	17.262	2572	2579	2589	rBV2	35135	90222	2.33%	0.331%
42	18.392	2763	2771	2785	rVB2	20806	63343	1.64%	0.232%

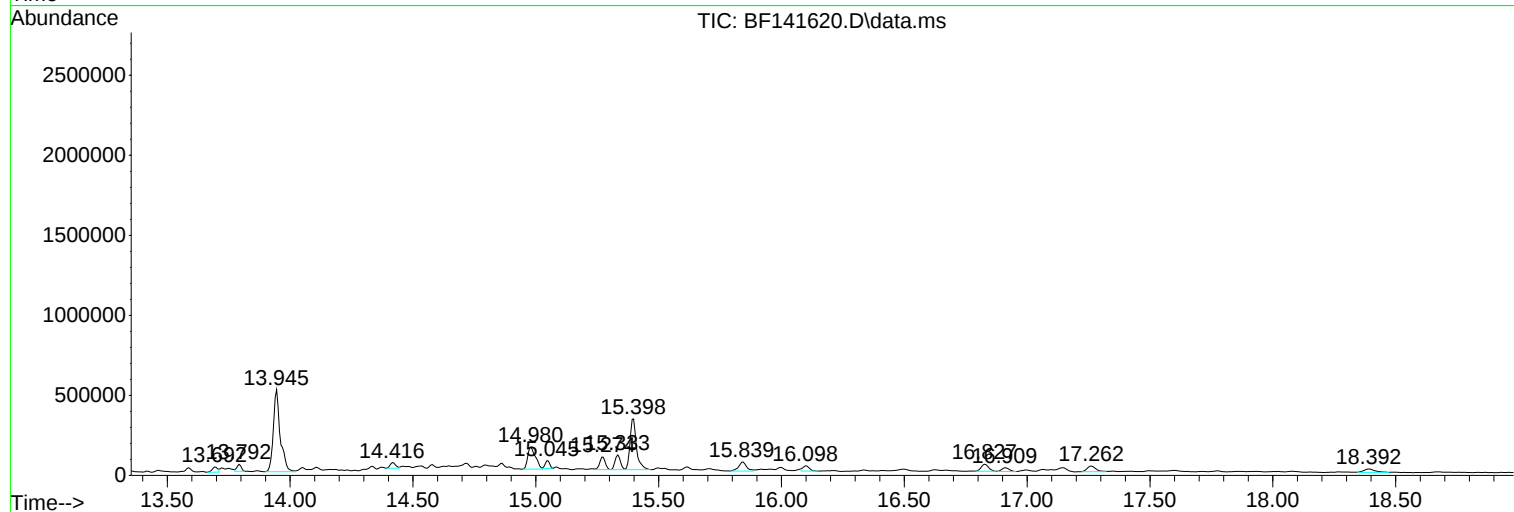
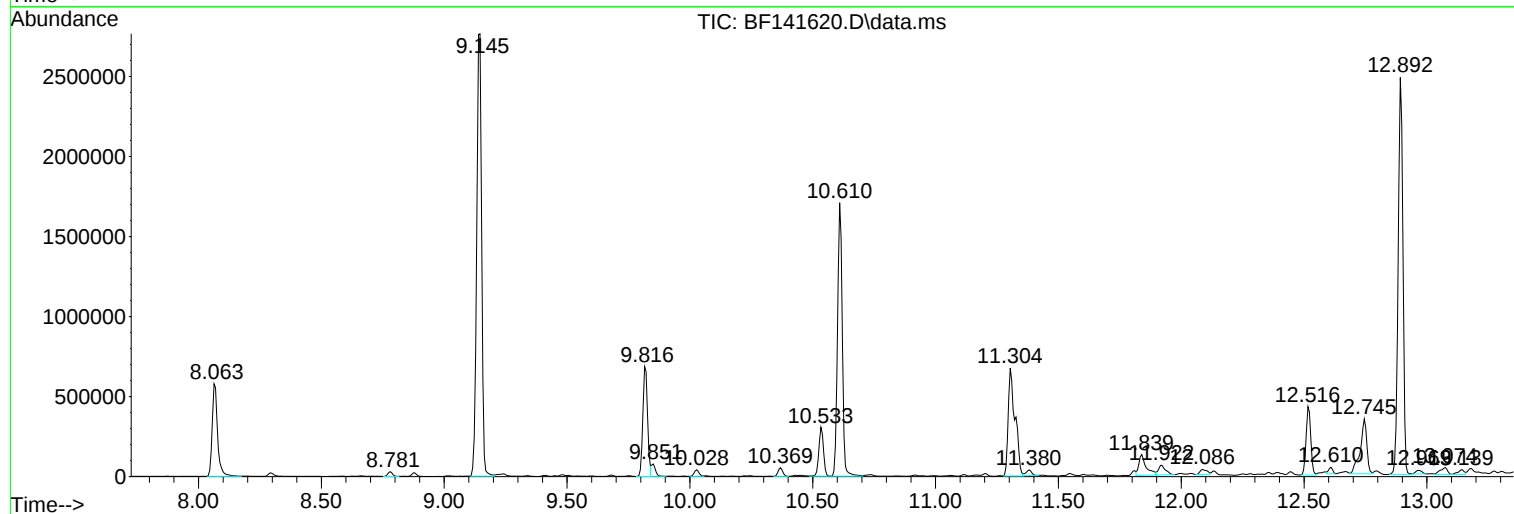
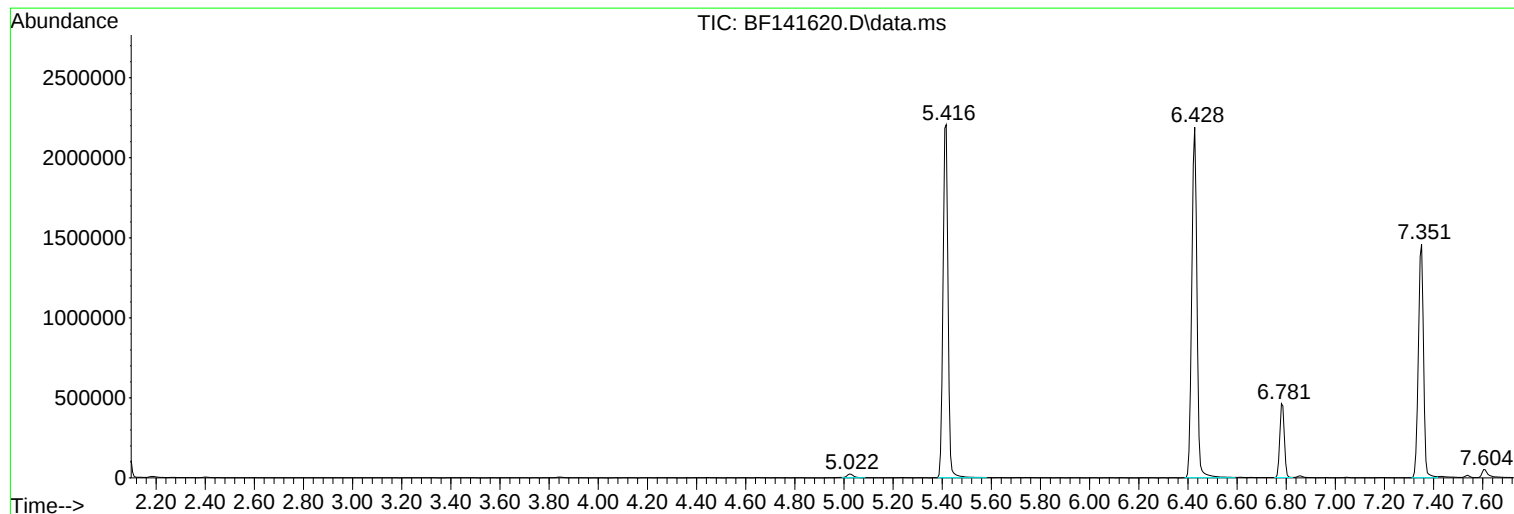
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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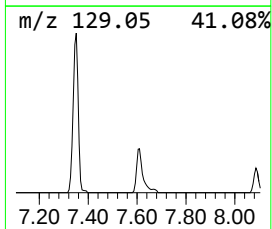
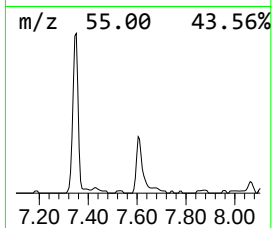
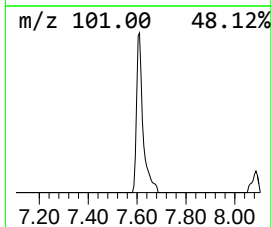
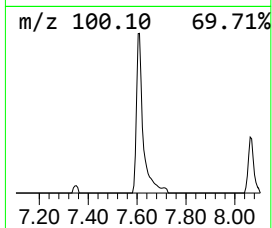
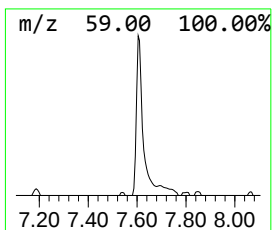
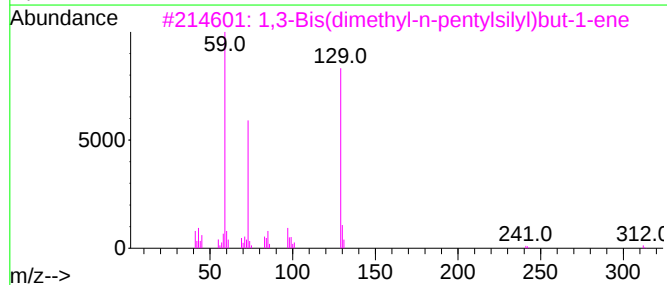
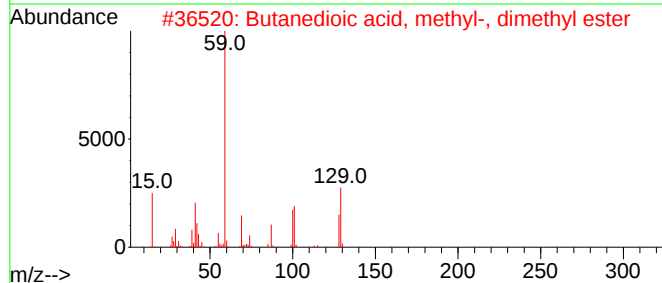
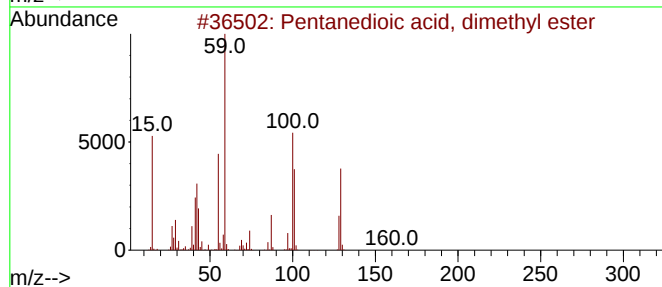
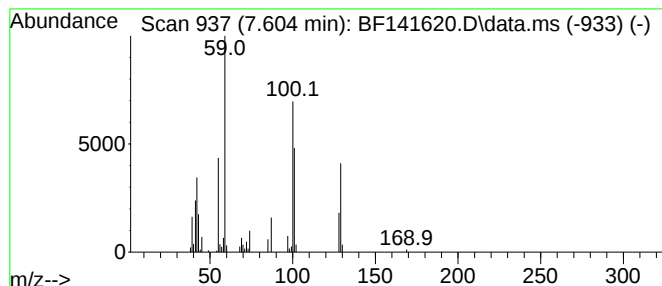
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.604	2.07 ng	90356	Naphthalene-d8	8.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	90
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	59
3			1,3-Bis(dimethyl-n-pentylsilyl)b...	312	C18H40Si2	136935-59-6	35
4			Butyric acid, 3-bromo-, methyl e...	180	C5H9BrO2	021249-59-2	32
5			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	27



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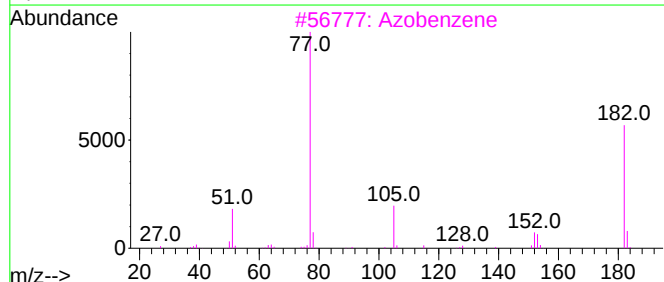
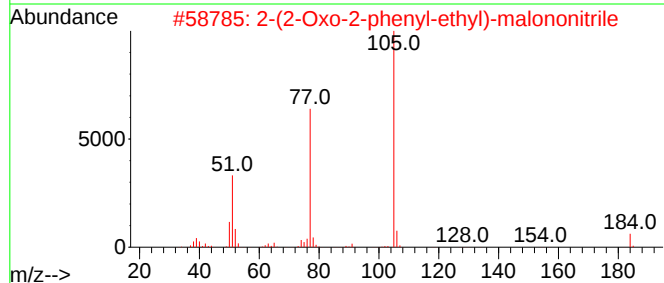
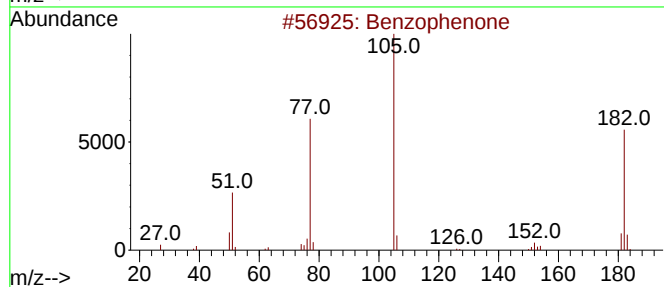
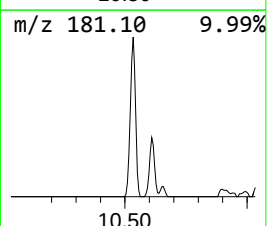
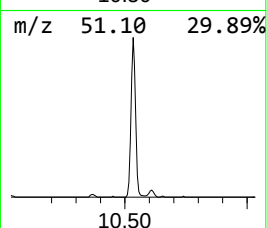
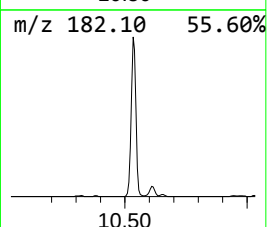
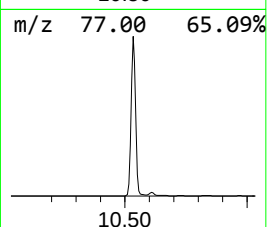
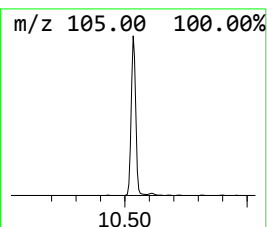
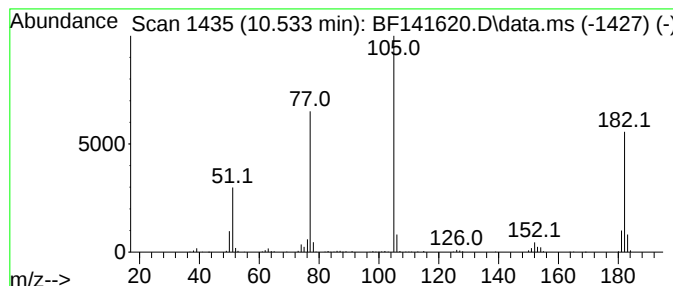
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.533	8.64 ng	396766	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
3			Azobenzene	182	C12H10N2	000103-33-3	52
4			Benzoylformic acid	150	C8H6O3	000611-73-4	49
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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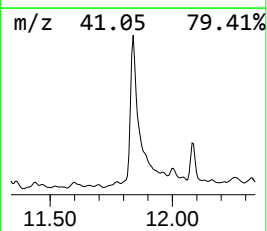
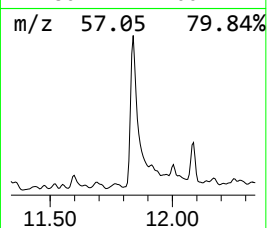
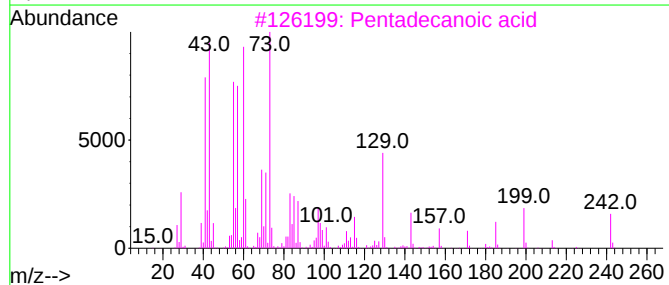
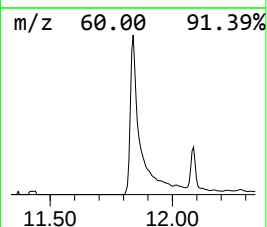
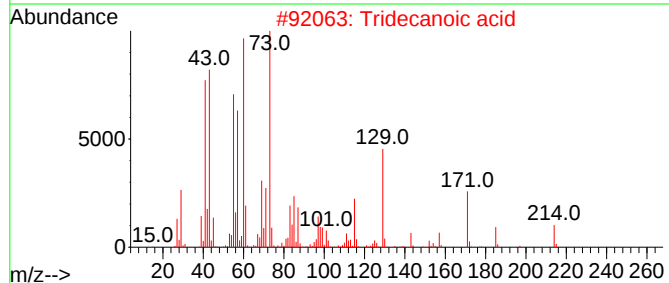
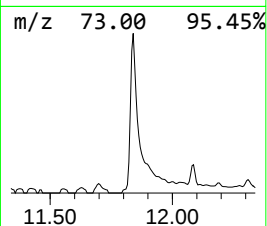
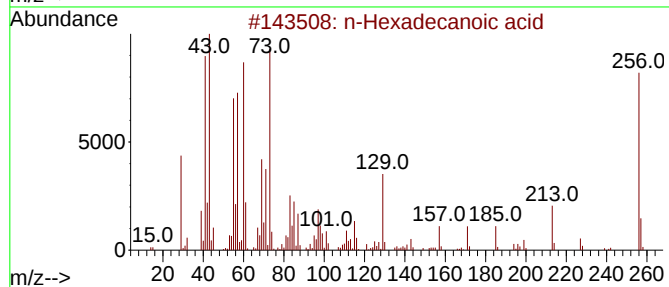
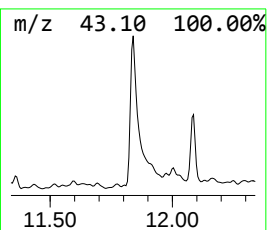
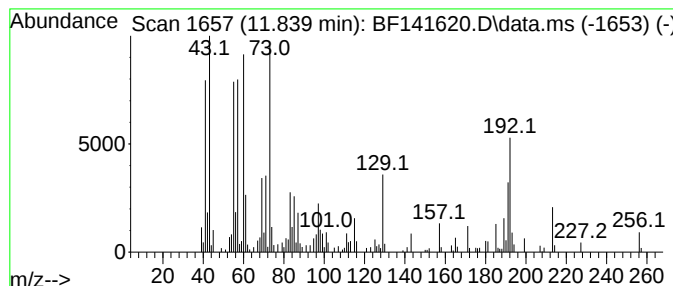
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.03 ng	264419	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	60



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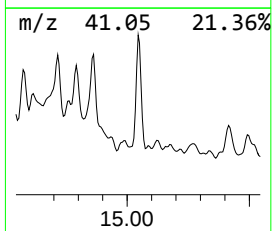
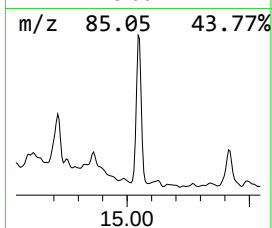
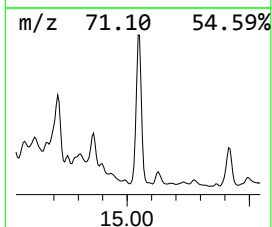
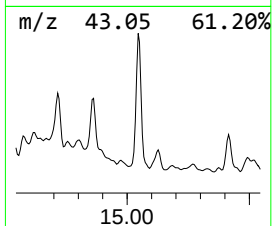
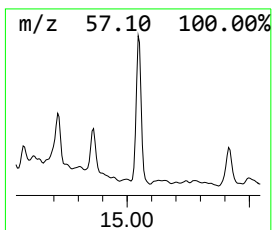
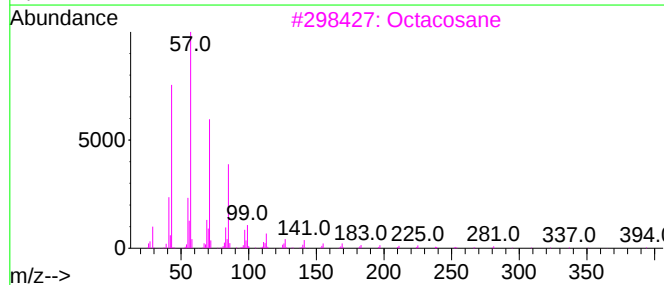
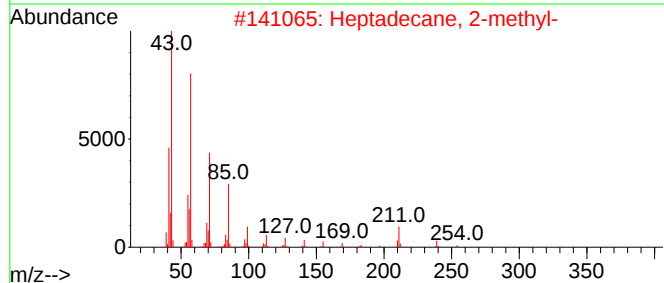
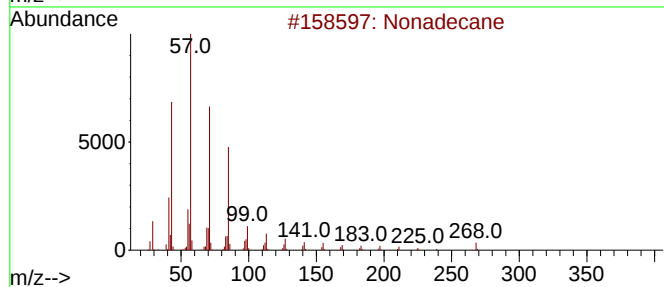
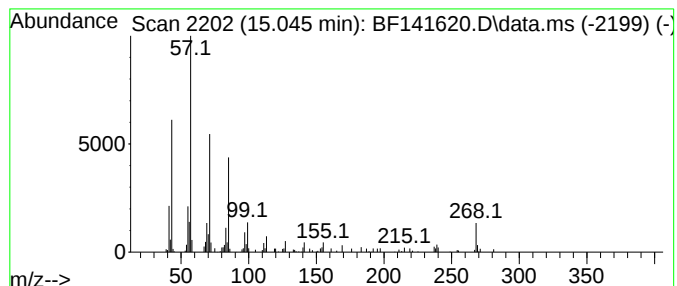
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Peak Number 4 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	2.18 ng	63088	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	91
3			Octacosane	394	C28H58	000630-02-4	87
4			Tetracosane	338	C24H50	000646-31-1	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



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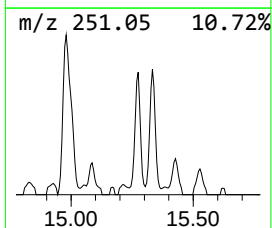
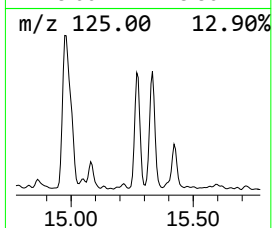
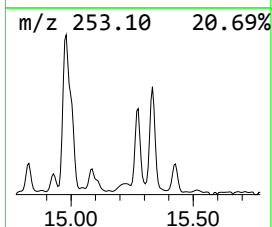
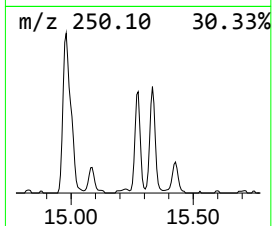
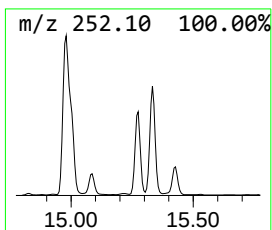
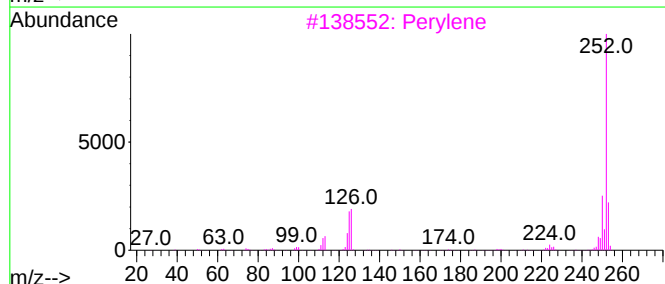
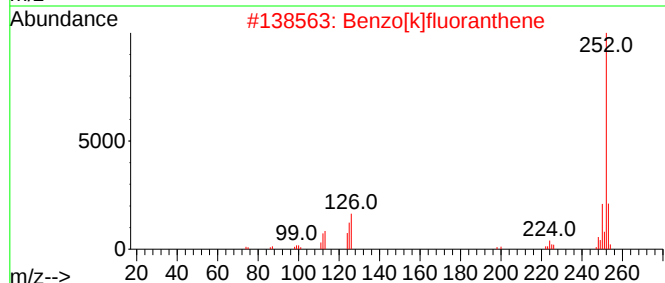
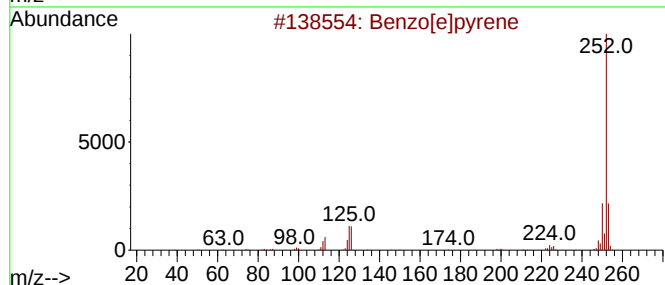
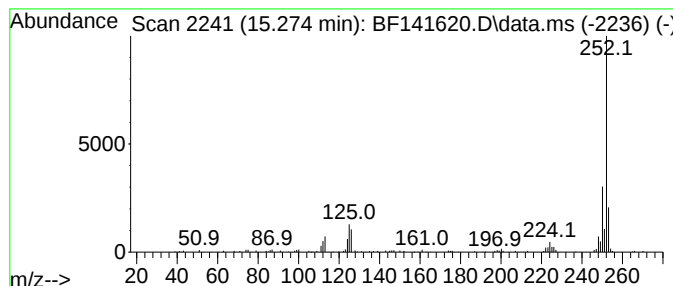
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.274	4.27 ng	123702	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	97
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Perylene	252	C20H12	000198-55-0	95
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021325\
Data File : BF141620.D
Acq On : 13 Feb 2025 17:42
Operator : RC/JU
Sample : Q1353-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
346

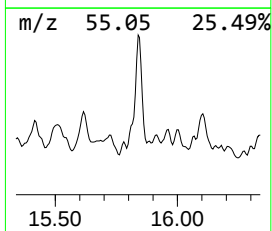
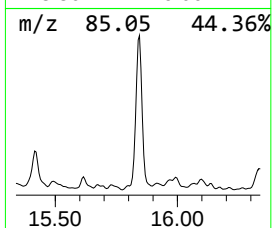
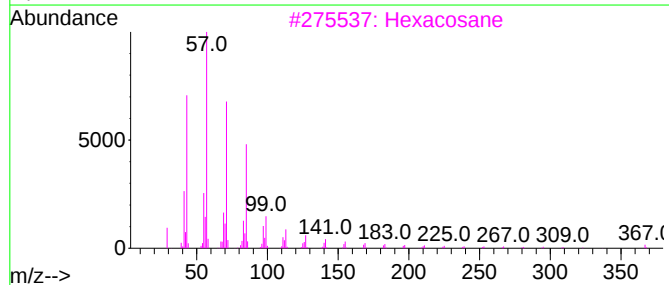
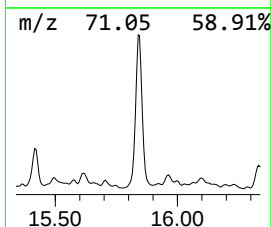
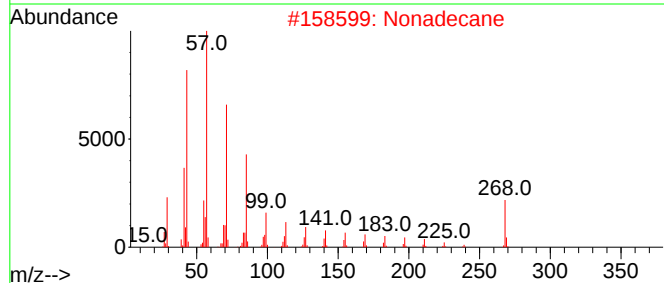
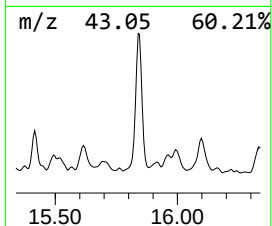
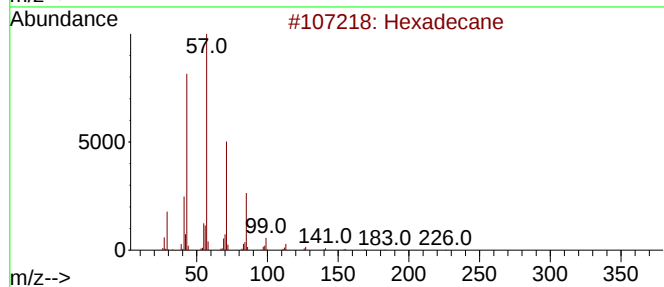
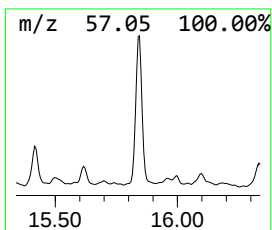
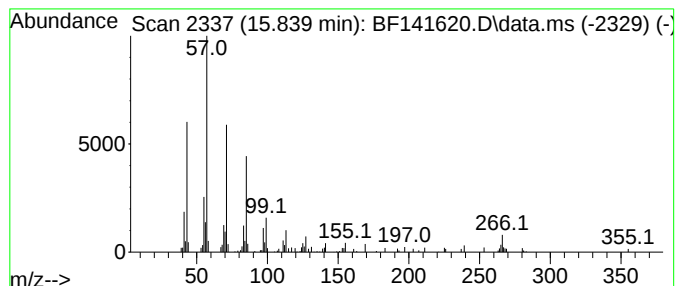
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	4.41 ng	127908	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Nonadecane	268	C19H40	000629-92-5	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021325\
Data File : BF141620.D
Acq On : 13 Feb 2025 17:42
Operator : RC/JU
Sample : Q1353-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
346

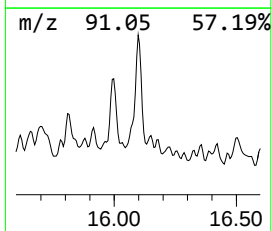
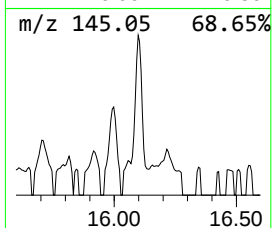
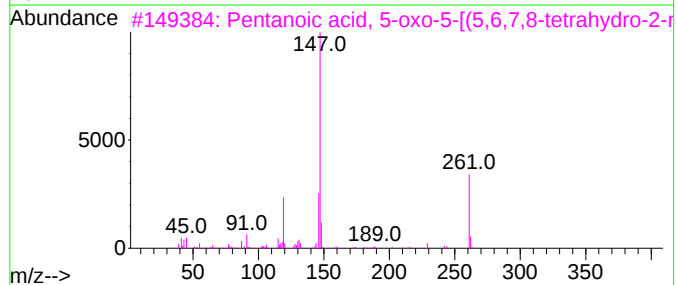
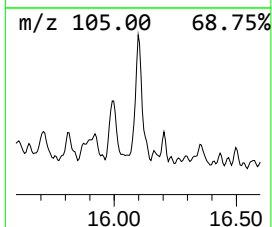
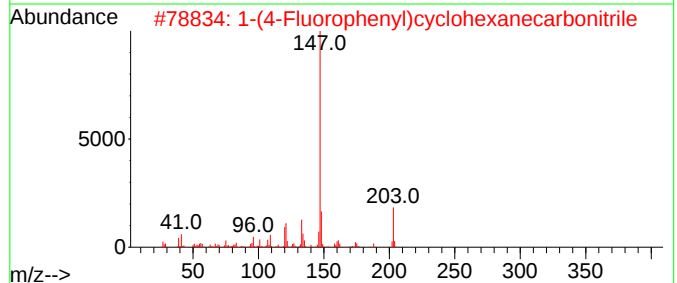
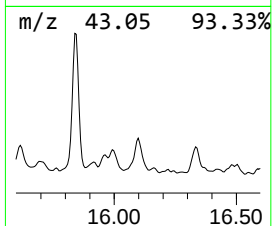
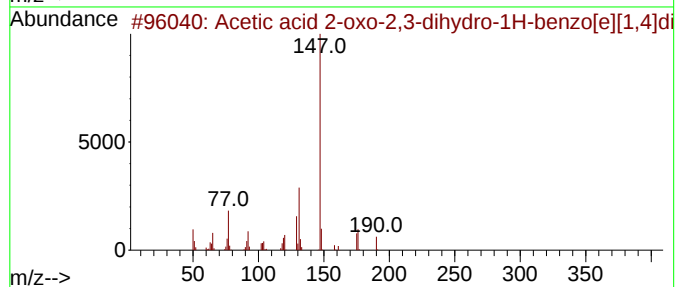
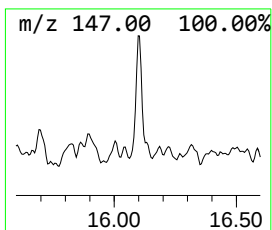
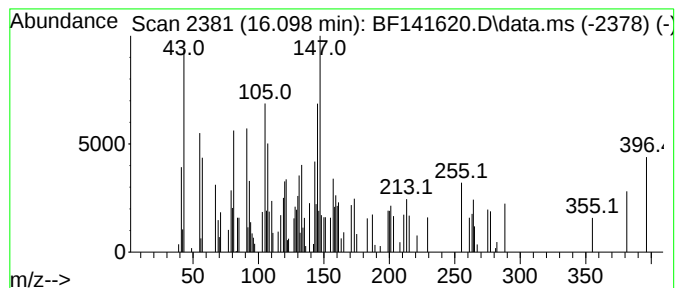
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.098 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.098	2.01 ng	58313	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid 2-oxo-2,3-dihydro-1H...	218	C11H10N2O3	016780-58-8	10
2			1-(4-Fluorophenyl)cyclohexanecar...	203	C13H14FN	071486-43-6	10
3			Pentanoic acid, 5-oxo-5-[(5,6,7,...	261	C15H19NO3	1000337-45-4	10
4			Benzene, (1-butyloctyl)-	246	C18H30	002719-63-3	10
5			1,3-dithiolan-2-one, 4-(iodometh...	274	C5H7IOS2	1010397-03-4	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021325\
Data File : BF141620.D
Acq On : 13 Feb 2025 17:42
Operator : RC/JU
Sample : Q1353-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
346

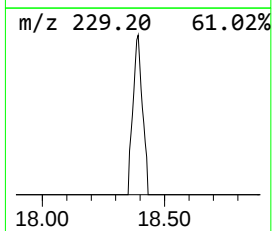
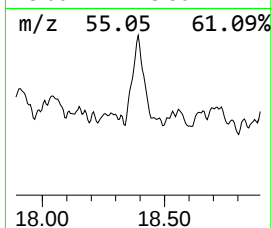
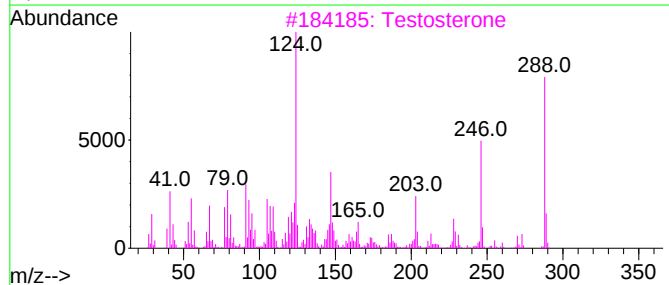
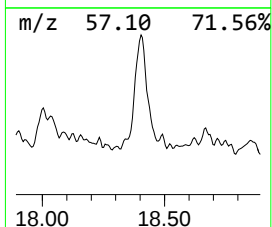
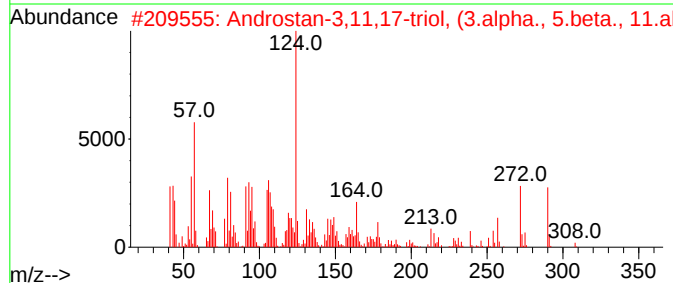
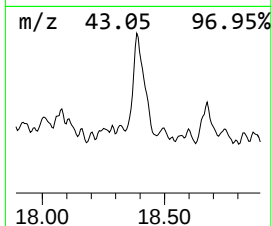
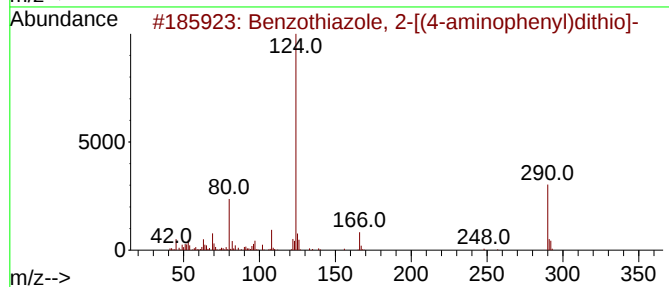
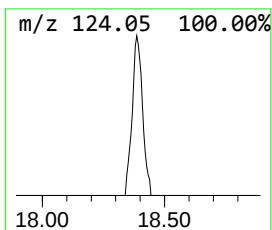
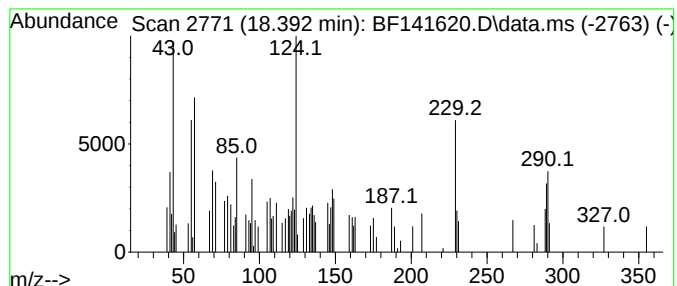
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.392 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.392	2.19 ng	63343	Perylene-d12	15.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzothiazole, 2-[(4-aminophenyl)...	290	C13H10N2S3	159357-92-3	27
2			Androstan-3,11,17-triol, (3.alpha...	308	C19H32O3	004484-95-1	22
3			Testosterone	288	C19H28O2	000058-22-0	22
4			Pregn-4-en-3-one, 20-hydroxy-, (...)	316	C21H32O2	000145-14-2	22
5			4-Methoxy-2-pyridinylamine	124	C6H8N2O	010201-73-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021325\
Data File : BF141620.D
Acq On : 13 Feb 2025 17:42
Operator : RC/JU
Sample : Q1353-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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	10.533	8.6	ng	396766	3	9.816	918636	20.0
n-Hexadecanoic ...	11.839	4.0	ng	264419	4	11.304	1311040	20.0
Nonadecane	15.045	2.2	ng	63088	6	15.398	579444	20.0
Benzo[e]pyrene	15.274	4.3	ng	123702	6	15.398	579444	20.0
Hexadecane	15.839	4.4	ng	127908	6	15.398	579444	20.0
unknown16.098	16.098	2.0	ng	58313	6	15.398	579444	20.0
unknown18.392	18.392	2.2	ng	63343	6	15.398	579444	20.0