LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

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

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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	13	26	rVB	1173065	1864823	49.25%	5.714%
2	5.110	509	513	519	rVB2	33303	53879	1.42%	0.165%
3	5.498	573	579	584	rBV	2844702	3713108	98.07%	11.378%
4	6.498	743	749	759	rBV	2781960	3786299	100.00%	11.602%
5	6.887	809	815	821	rVB	932841	1167396	30.83%	3.577%
6	7.440	901	909	914	rBV	1876660	2417207	63.84%	7.407%
7	7.692	948	952	958	rVB	91494	113787	3.01%	0.349%
8	8.163	1026	1032	1039	rBV	1182559	1510343	39.89%	4.628%
9	8.375	1063	1068	1076	rVB2	39940	58674	1.55%	0.180%
10	8.875	1146	1153	1158	rVB	53400	67758	1.79%	0.208%
11	8.975	1166	1170	1174	rBV	46299	54035	1.43%	0.166%
12	9.239	1209	1215	1220	rBV	2870613	3692003	97.51%	11.313%
13	9.322	1224	1229	1235	rVB2	31544	53959	1.43%	0.165%
14	9.575	1265	1272	1274	rBV	36053	52945	1.40%	0.162%
15	9.916	1324	1330	1335	rBV	1267609	1583722	41.83%	4.853%
16	10.628	1445	1451	1458	rBV	307754	387402	10.23%	1.187%
17	10.698	1458	1463	1478	rVV	1700314	2295535	60.63%	7.034%
18	10.828	1480	1485	1492	rVB2	47847	81799	2.16%	0.251%
19	11.269	1554	1560	1563	rBV3	27300	46927	1.24%	0.144%
20	11.404	1577	1583	1590	rBV	1082434	1549322	40.92%	4.747%
21	11.628	1616	1621	1628	rBV2	34722	66861	1.77%	0.205%
22	11.927	1664	1672	1680	rBV2	357903	603851	15.95%	1.850%
23	11.998	1680	1684	1689	rVV2	62673	135846	3.59%	0.416%
24	12.086	1692	1699	1705	rVB2	69049	186635	4.93%	0.572%
25	12.492	1763	1768	1773	rVB3	60057	116524	3.08%	0.357%
26	12.610	1784	1788	1794	rBV	159439	210613	5.56%	0.645%
27	12.710	1801	1805	1813	rBV2	58413	103736	2.74%	0.318%
28	12.839	1822	1827	1834	rBV2	145054	260460	6.88%	0.798%
29	12.986	1846	1852	1859	rVB	2004684	2598058	68.62%	7.961%
30	13.169	1880	1883	1889	rVB4	34463	53731	1.42%	0.165%
31	13.886	2000	2005	2014	rVB2	139274	243634	6.43%	0.747%
32	14.033	2025	2030	2044	rVB2	958697	1490757	39.37%	4.568%
33	15.074	2203	2207	2217	rVB	158723	318578	8.41%	0.976%
34	15.380	2255	2259	2265	rVB	94695	140356	3.71%	0.430%
35	15.439	2265	2269	2275	rVV	97908	153298	4.05%	0.470%
36	15.510	2275	2281	2293	rVB	859658	1401178	37.01%	4.293%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

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

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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

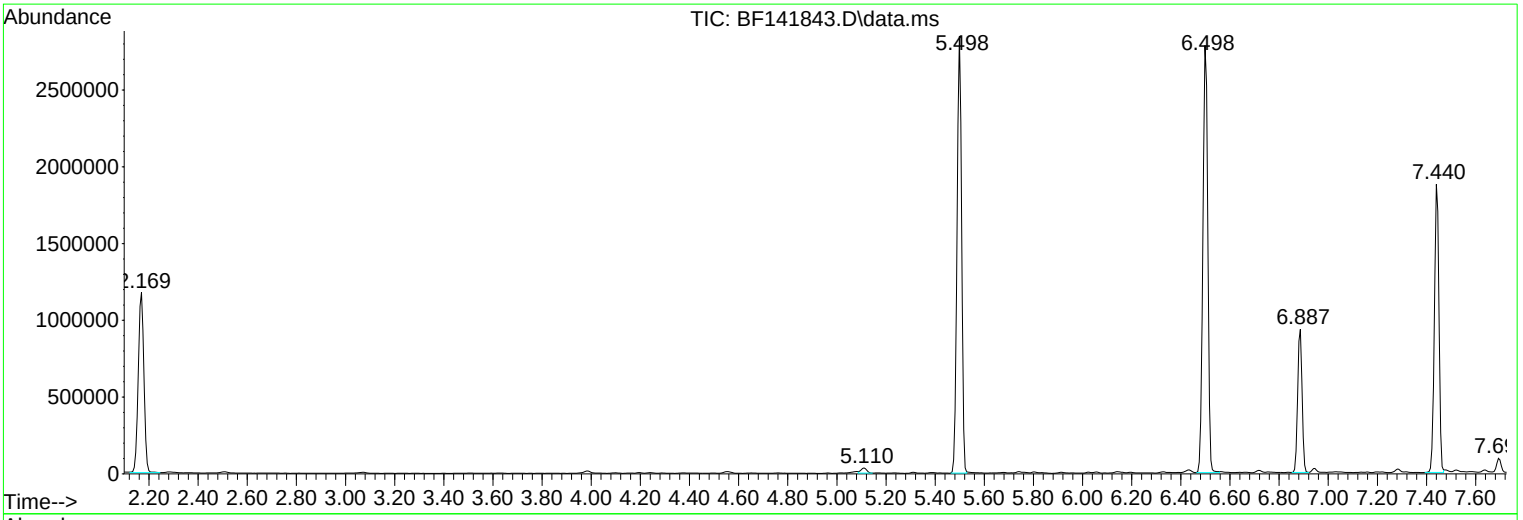
Sum of corrected areas: 32635039

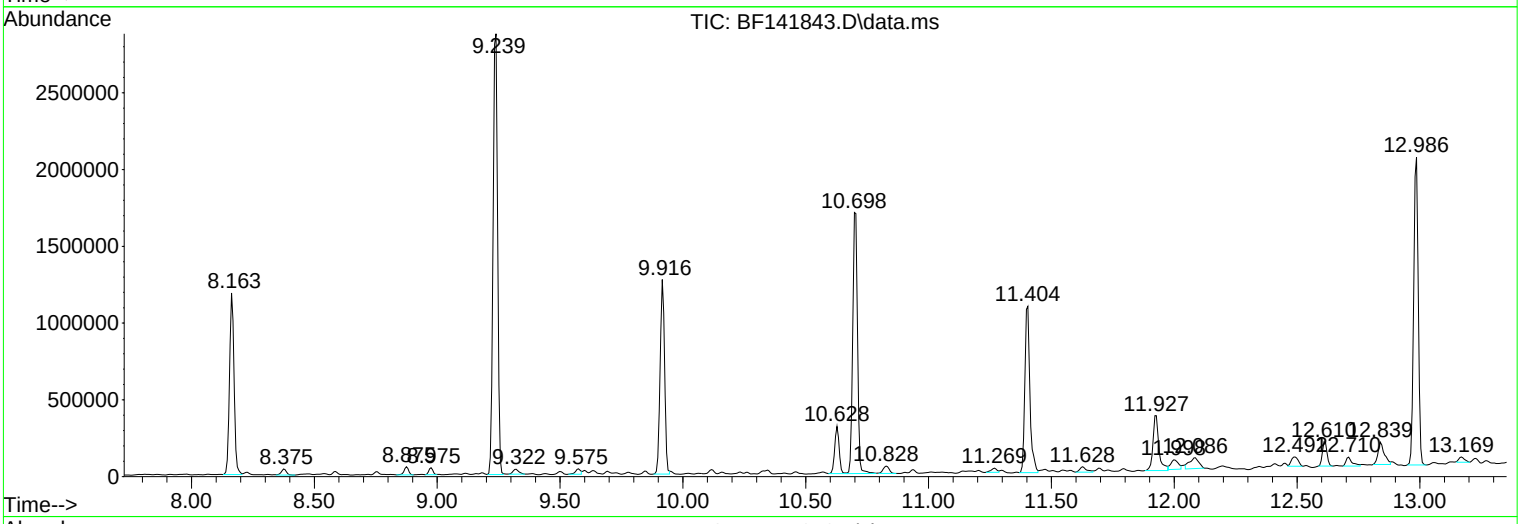
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

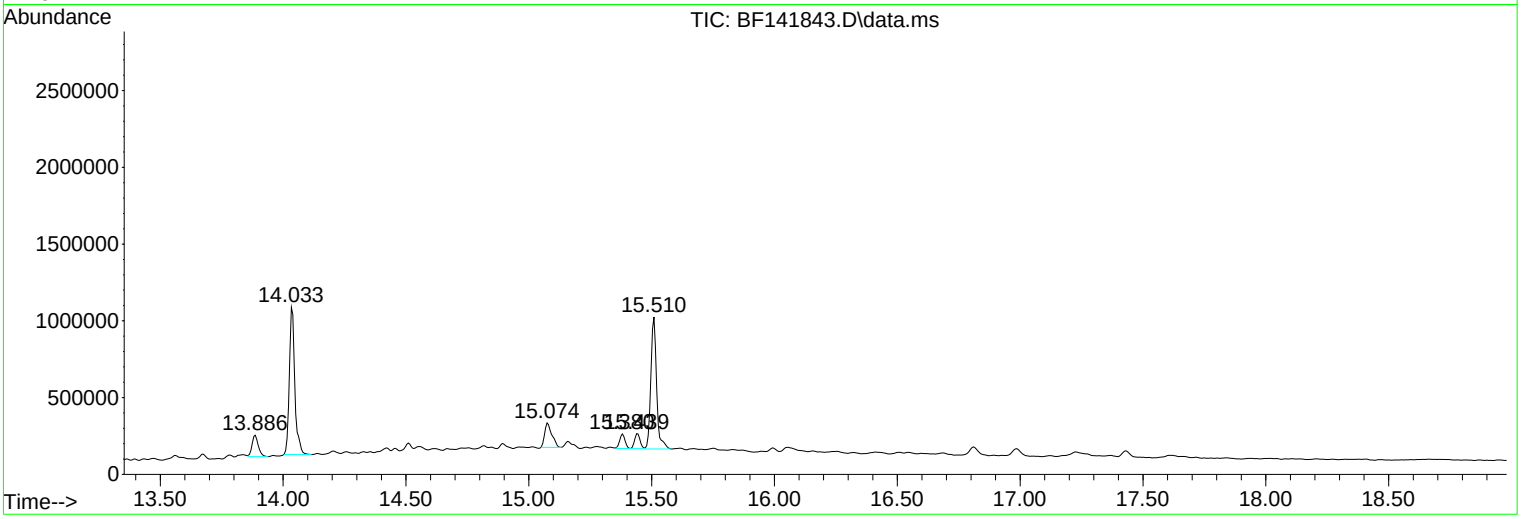
Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

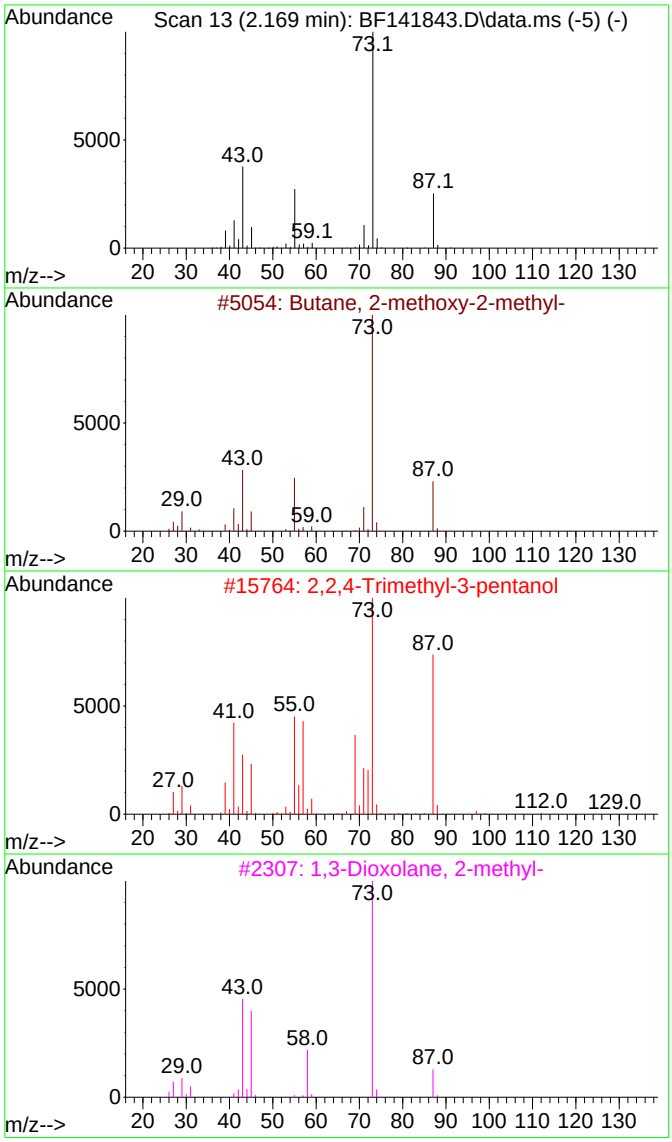
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

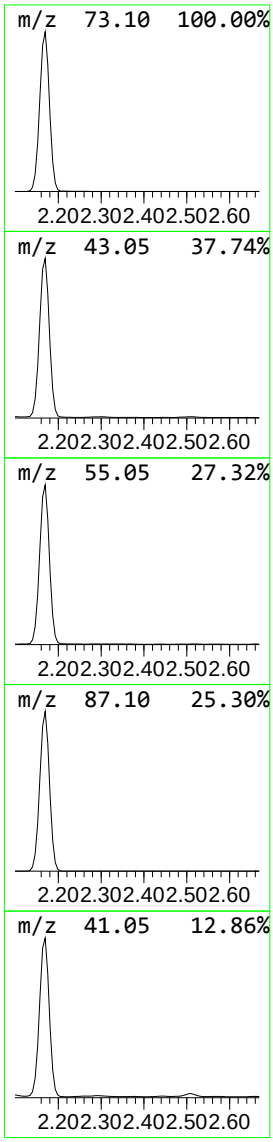
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	31.95 ng	1864820	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

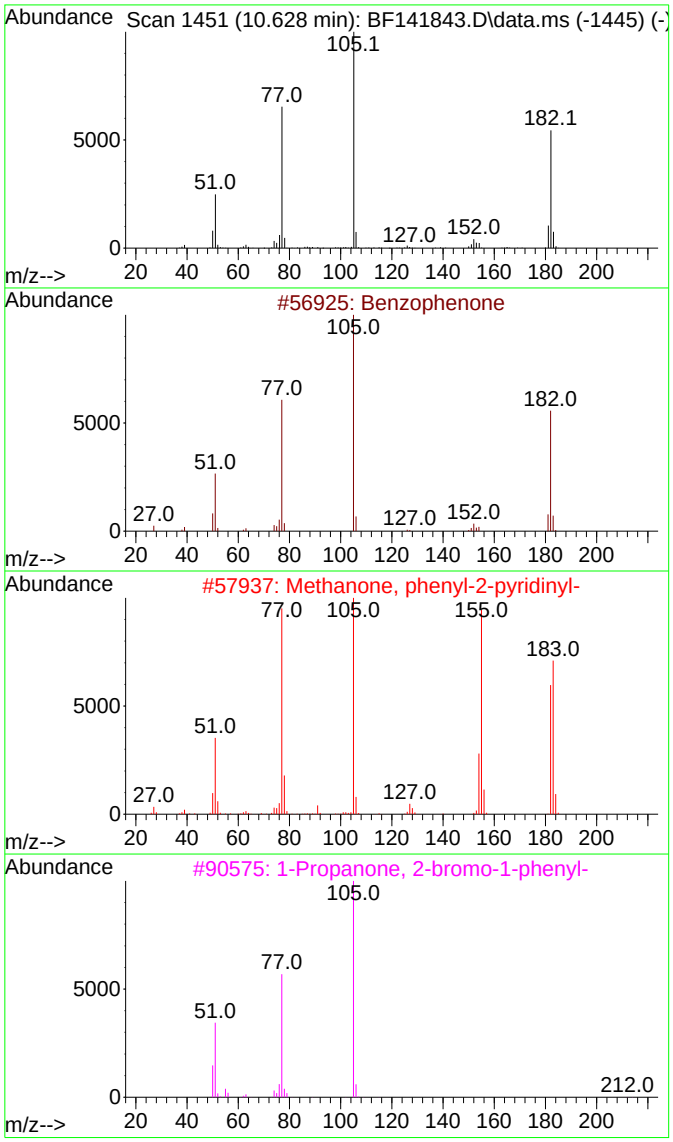
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

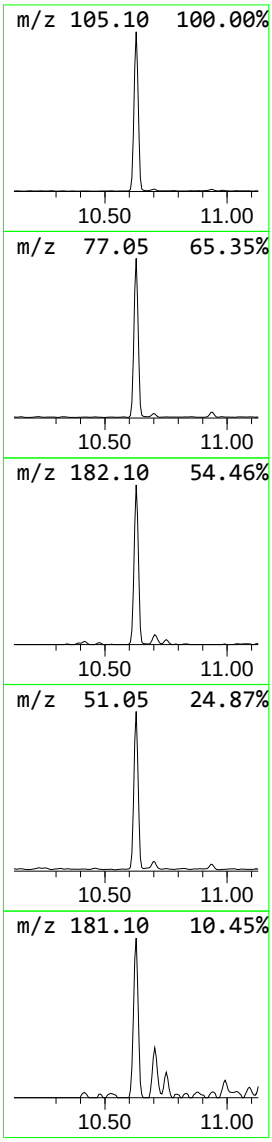
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	4.89 ng	387402	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	72
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

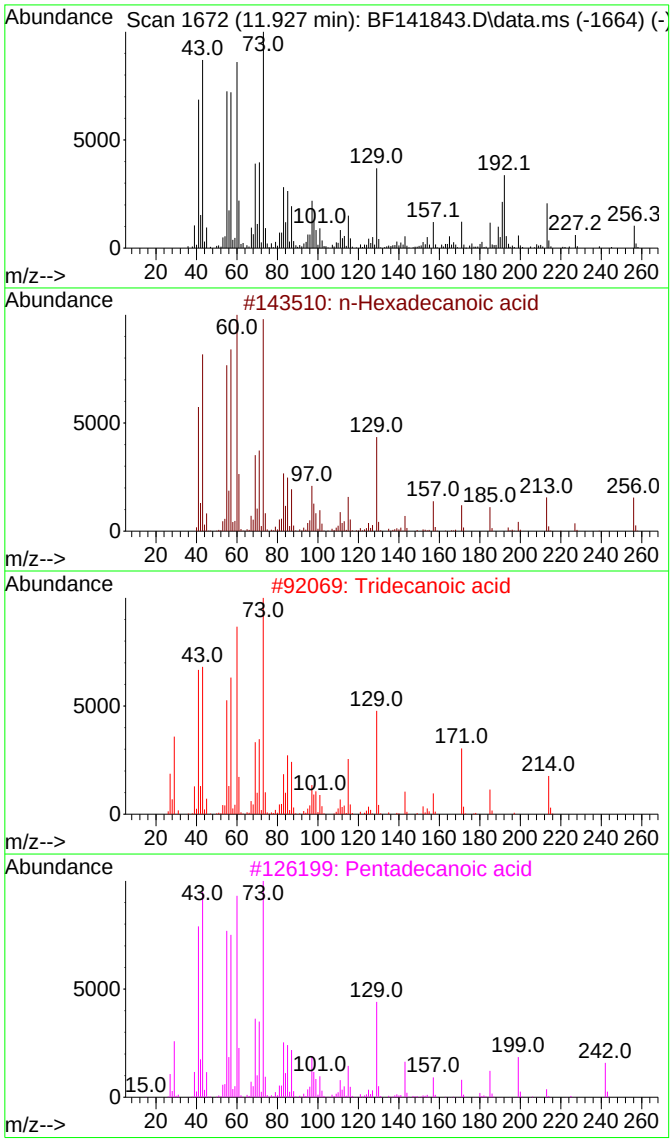
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

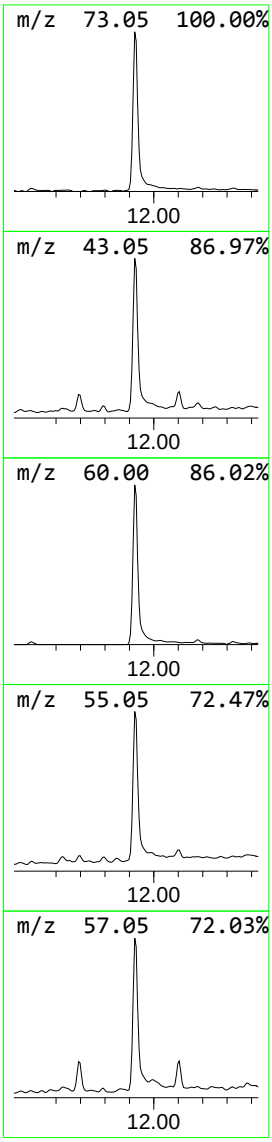
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	7.80 ng	603851	Phenanthrene-d10	11.404

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

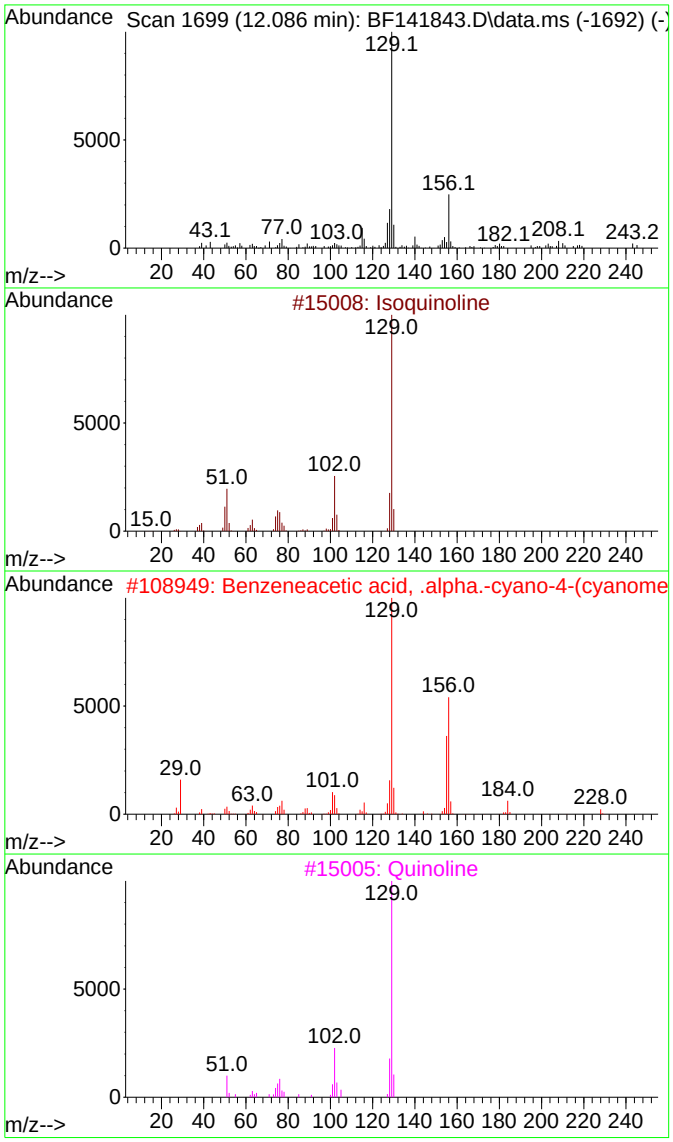
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

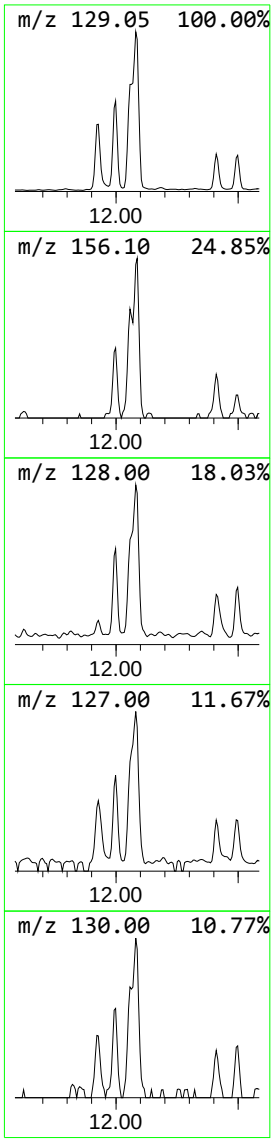
****

Peak Number 4 Isoquinoline Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.086	2.41 ng	186635	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoquinoline	129	C9H7N	000119-65-3	58
2	Benzeneacetic acid, .alpha.-cyan...	228	C13H12N2O2	134882-04-5	56
3	Quinoline	129	C9H7N	000091-22-5	53
4	Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	50
5	1-Deuteronaphthalene	129	C10H7D	000875-62-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

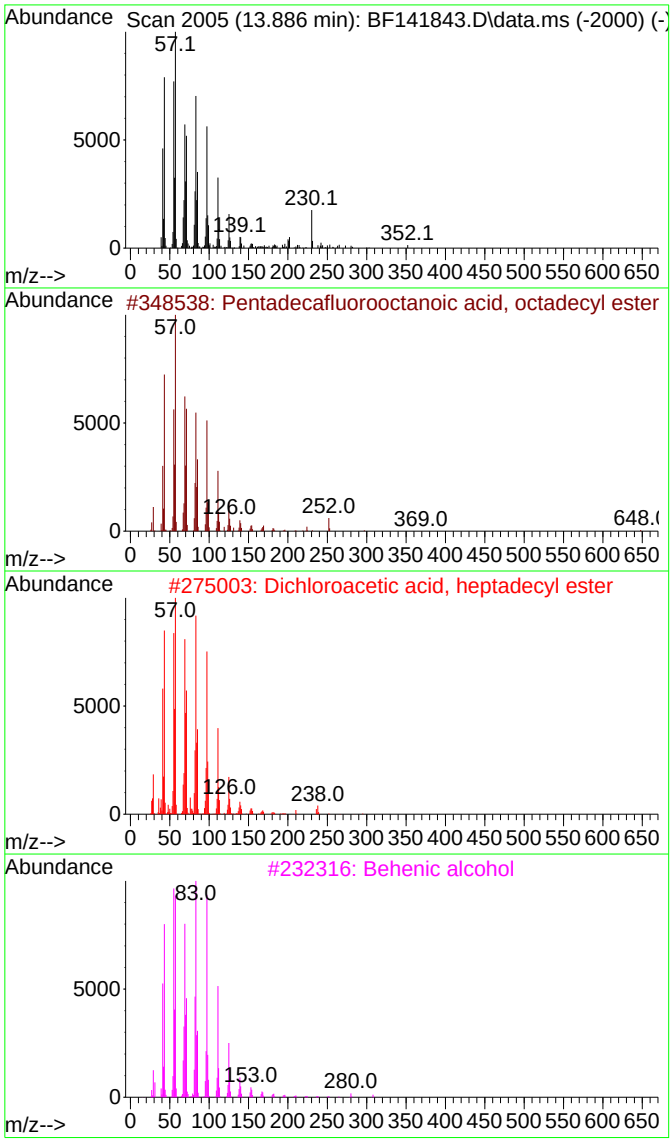
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

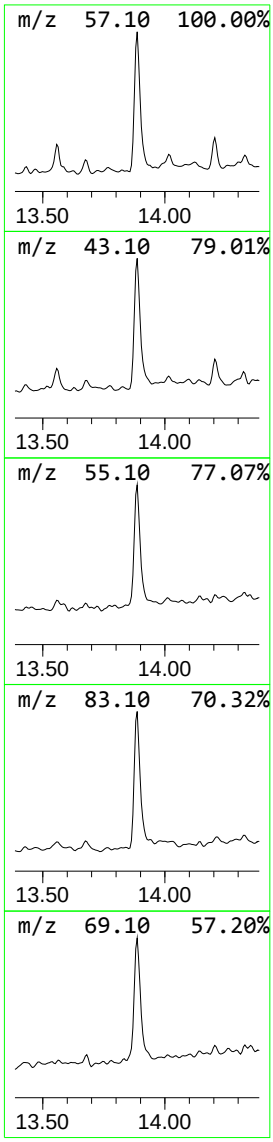
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.27 ng	243634	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





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Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

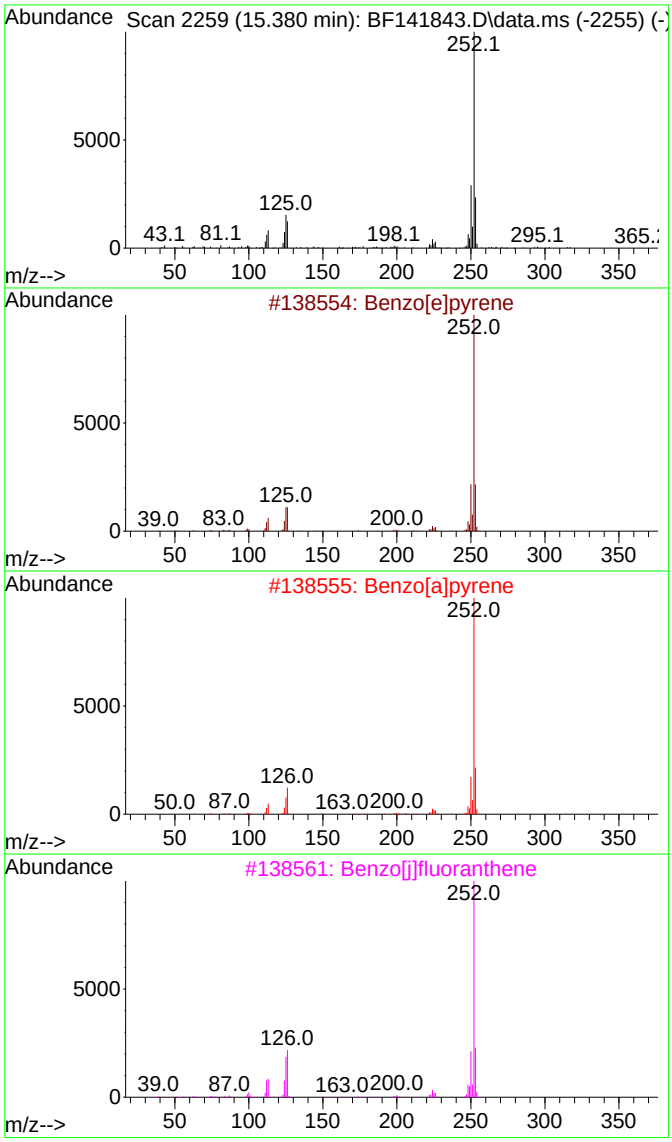
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

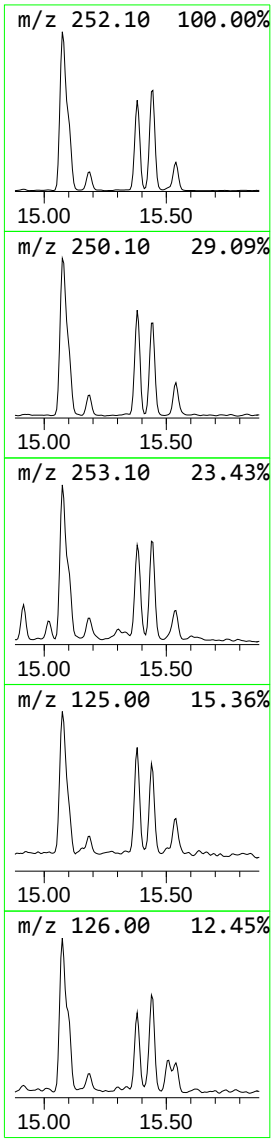
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	2.00 ng	140356	Perylene-d12	15.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	94
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030525\
Data File : BF141843.D
Acq On : 05 Mar 2025 14:52
Operator : RC/JU
Sample : Q1488-09
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-SB01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.169	31.9	ng	1864820	1	6.887	1167400	20.0
Benzophenone	10.628	4.9	ng	387402	3	9.916	1583720	20.0
n-Hexadecanoic ...	11.928	7.8	ng	603851	4	11.404	1549320	20.0
Isoquinoline	12.086	2.4	ng	186635	4	11.404	1549320	20.0
Pentadecafluoro...	13.886	3.3	ng	243634	5	14.033	1490760	20.0
Benzo[e]pyrene	15.380	2.0	ng	140356	6	15.510	1401180	20.0