LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070125\
Data File : BF142955.D
Acq On : 01 Jul 2025 18:00
Operator : RC/JU
Sample : Q2458-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-60

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-BF061925.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142955.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	482	490	504	rBV	42024	63672	6.59%	0.825%
2	5.487	555	560	578	rBV	449093	595796	61.65%	7.719%
3	6.498	727	732	758	rBV	422616	543498	56.24%	7.042%
4	6.875	791	796	803	rBV	173477	220985	22.87%	2.863%
5	7.434	886	891	903	rBV	280193	347532	35.96%	4.503%
6	8.157	1006	1014	1021	rBV	205747	256712	26.56%	3.326%
7	9.228	1191	1196	1202	rBV	542018	685059	70.88%	8.876%
8	9.310	1206	1210	1215	rVV3	7920	10980	1.14%	0.142%
9	9.622	1259	1263	1270	rBV3	12672	22149	2.29%	0.287%
10	9.775	1285	1289	1293	rBV	24118	30643	3.17%	0.397%
11	9.833	1293	1299	1303	rVB3	6639	12352	1.28%	0.160%
12	9.910	1307	1312	1317	rBV	230777	289442	29.95%	3.750%
13	10.333	1377	1384	1387	rBV3	9571	16075	1.66%	0.208%
14	10.557	1417	1422	1428	rBV2	11174	18300	1.89%	0.237%
15	10.622	1428	1433	1439	rVV	58591	78555	8.13%	1.018%
16	10.704	1440	1447	1457	rVV	370765	485872	50.27%	6.295%
17	10.822	1461	1467	1475	rVB	26231	46113	4.77%	0.597%
18	11.157	1517	1524	1529	rVB9	4404	11911	1.23%	0.154%
19	11.257	1537	1541	1544	rBV2	12749	18495	1.91%	0.240%
20	11.292	1544	1547	1553	rVB3	18583	27828	2.88%	0.361%
21	11.404	1560	1566	1575	rBV2	272363	442294	45.77%	5.730%
22	11.475	1575	1578	1581	rVV	14343	19351	2.00%	0.251%
23	11.510	1582	1584	1590	rVB6	5966	9919	1.03%	0.129%
24	11.639	1602	1606	1610	rBV4	11191	16495	1.71%	0.214%
25	11.686	1610	1614	1619	rVB2	13817	18506	1.91%	0.240%
26	11.927	1647	1655	1662	rBV2	115418	204314	21.14%	2.647%
27	12.016	1666	1670	1677	rVB	32744	61379	6.35%	0.795%
28	12.092	1680	1683	1687	rBV	12573	16352	1.69%	0.212%
29	12.198	1698	1701	1704	rBV	11588	14885	1.54%	0.193%
30	12.227	1704	1706	1712	rVB4	14180	16447	1.70%	0.213%
31	12.345	1721	1726	1729	rBV3	8894	17959	1.86%	0.233%
32	12.380	1729	1732	1739	rVB2	11452	18362	1.90%	0.238%
33	12.451	1741	1744	1747	rBV	21927	31892	3.30%	0.413%
34	12.486	1747	1750	1756	rVB5	20378	30598	3.17%	0.396%
35	12.545	1756	1760	1763	rBV	14667	21657	2.24%	0.281%
36	12.616	1768	1772	1777	rBV	261763	334083	34.57%	4.328%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070125\
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Acq On : 01 Jul 2025 18:00
Operator : RC/JU
Sample : Q2458-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-60

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-BF061925.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.710	1785	1788	1792	rBV2	24963	36457	3.77%	0.472%
38	12.845	1805	1811	1818	rBV	245431	379845	39.30%	4.921%
39	12.986	1830	1835	1843	rVB	739203	966443	100.00%	12.521%
40	13.069	1845	1849	1855	rBV2	24082	45809	4.74%	0.594%
41	13.280	1882	1885	1889	rBV2	31331	42589	4.41%	0.552%
42	14.045	2010	2015	2019	rBV2	336549	583850	60.41%	7.564%
43	15.104	2192	2195	2203	rVB	117947	231886	23.99%	3.004%
44	15.545	2266	2270	2289	rVB2	180101	375080	38.81%	4.860%

Sum of corrected areas: 7718421

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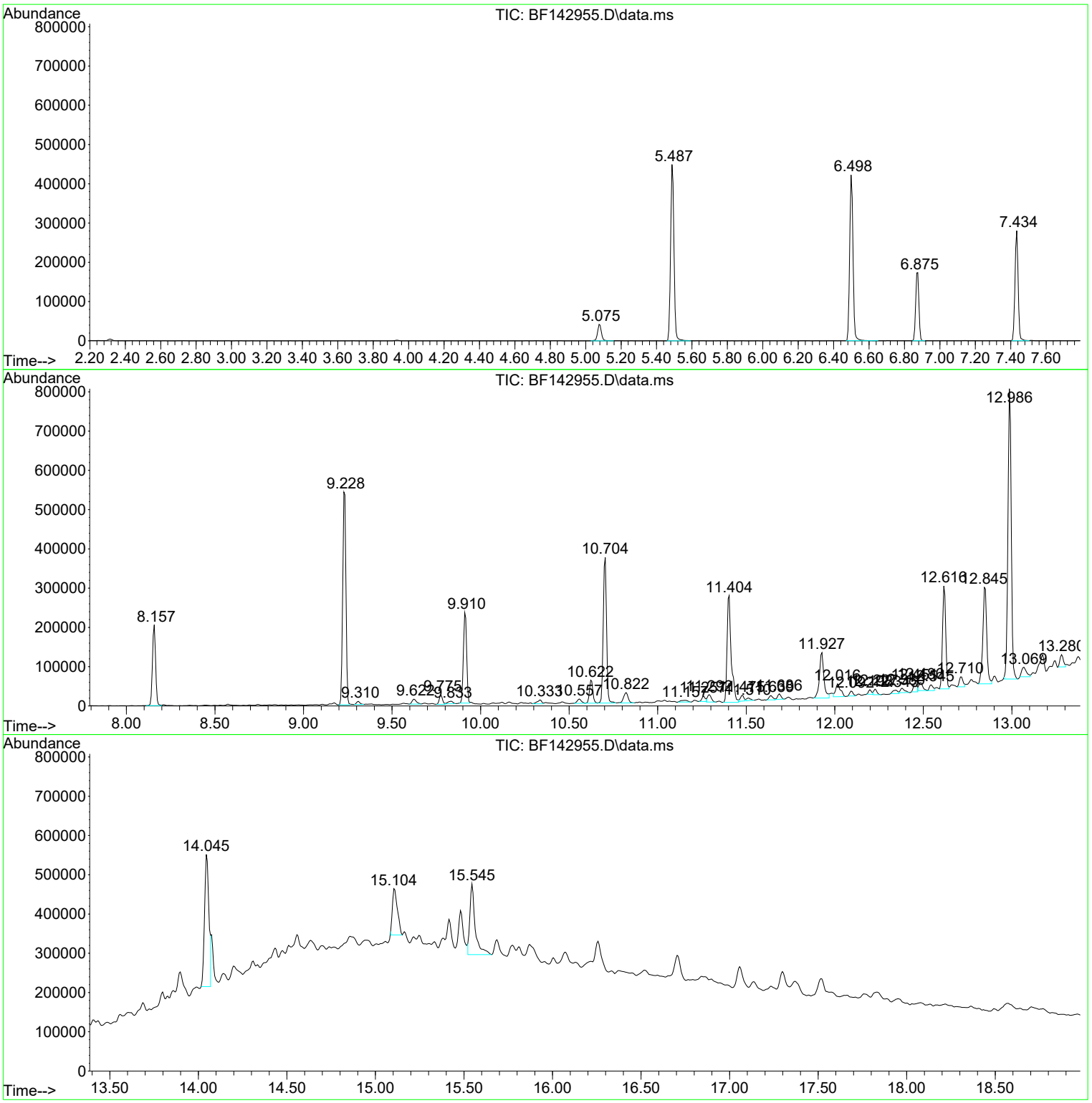
Instrument :
BNA_F
ClientSampleId :
TP-60

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.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\BF070125\
Data File : BF142955.D
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Operator : RC/JU
Sample : Q2458-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-60

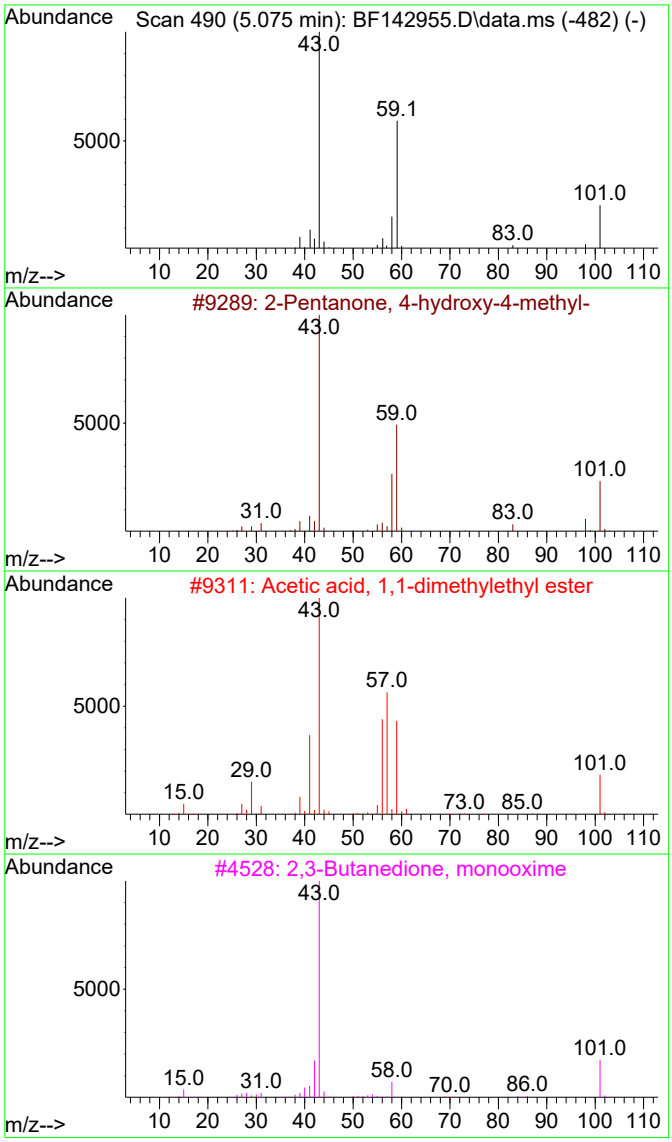
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

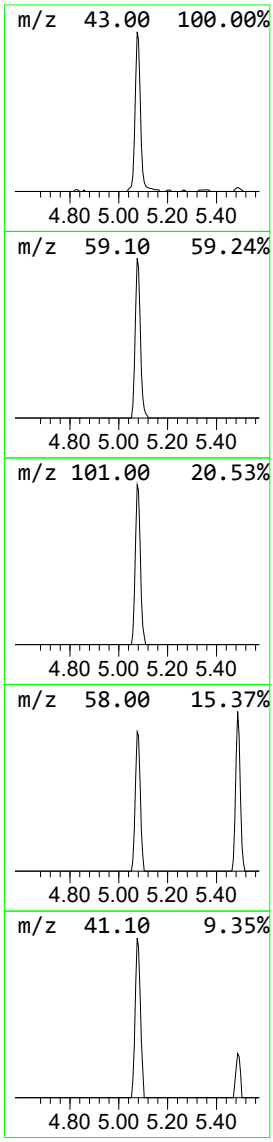
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.76 ng	63672	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	3-Octanol	130	C8H18O	000589-98-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





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Data File : BF142955.D
Acq On : 01 Jul 2025 18:00
Operator : RC/JU
Sample : Q2458-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-60

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

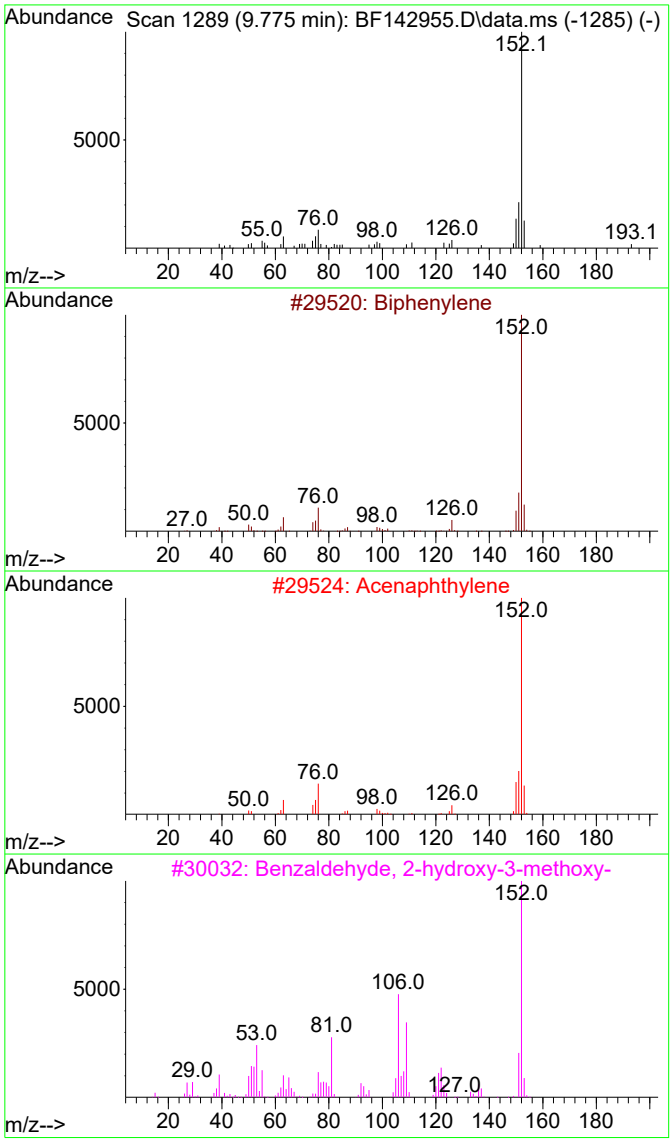
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

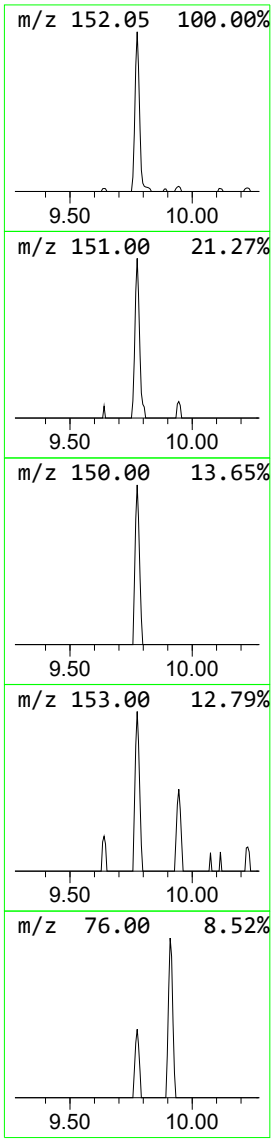
****

Peak Number 2 Biphenylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.775	2.12 ng	30643	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Biphenylene	152	C12H8	000259-79-0	87
2	Acenaphthylene	152	C12H8	000208-96-8	87
3	Benzaldehyde, 2-hydroxy-3-methoxy-	152	C8H8O3	000148-53-8	64
4	5,6-Dihydro-4-methylthieno(2,3-d...	152	C7H8N2S	092204-06-3	59
5	4-Methylbenzoic acid, (octahydro...	287	C18H25NO2	1000310-94-6	50





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Acq On : 01 Jul 2025 18:00
Operator : RC/JU
Sample : Q2458-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-60

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

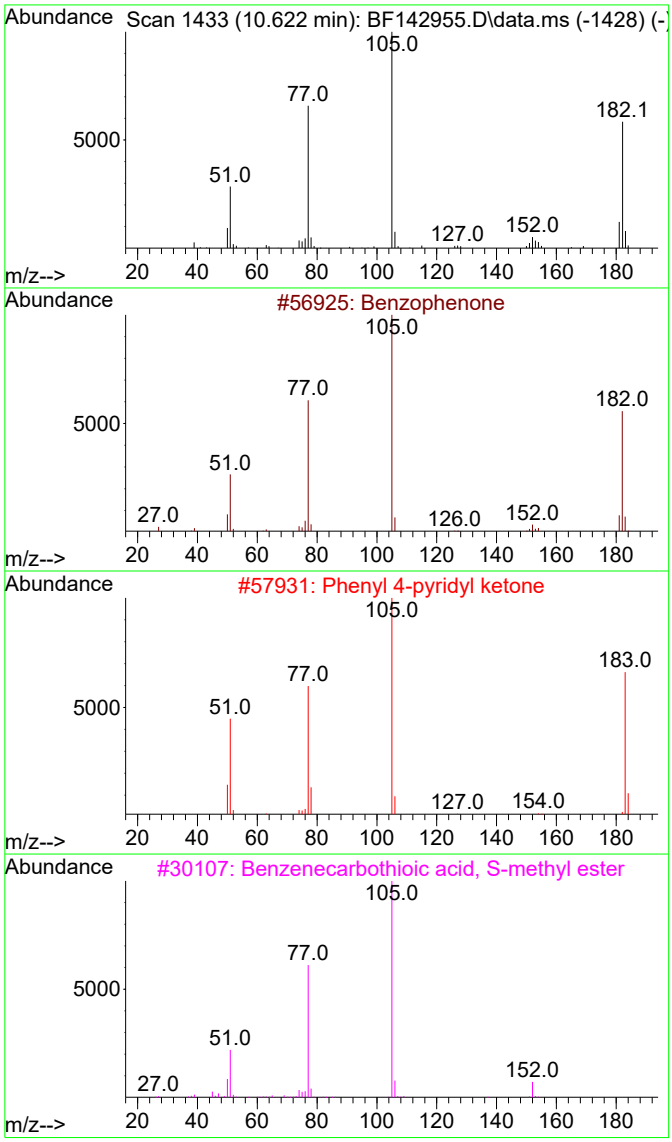
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

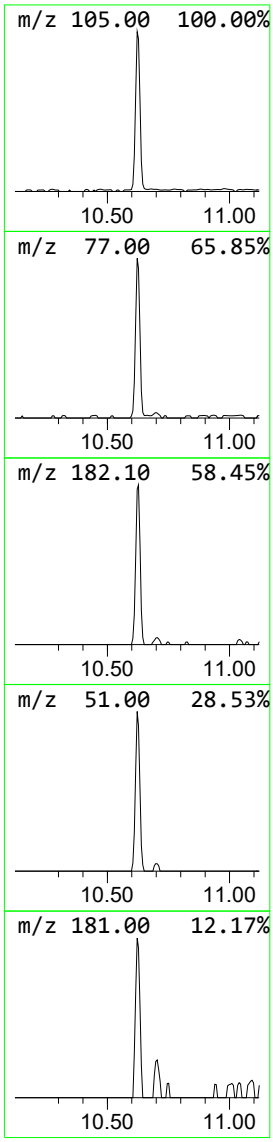
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	5.43 ng	78555	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	60
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
5	Benzoylformic acid	150	C8H6O3	000611-73-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070125\
Data File : BF142955.D
Acq On : 01 Jul 2025 18:00
Operator : RC/JU
Sample : Q2458-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-60

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

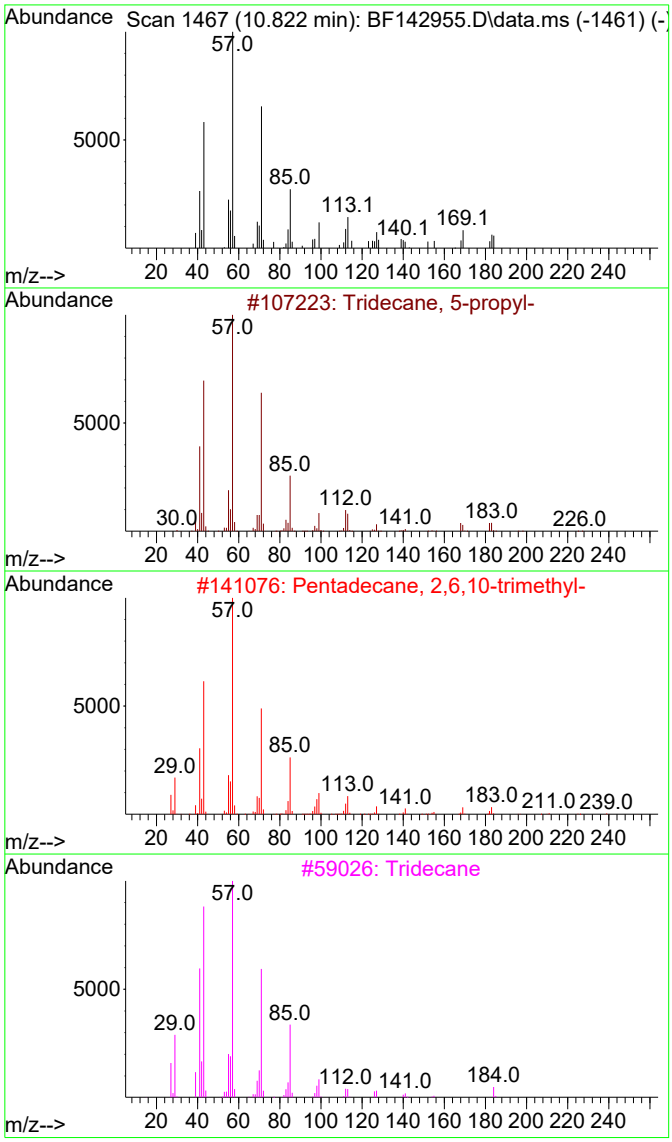
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

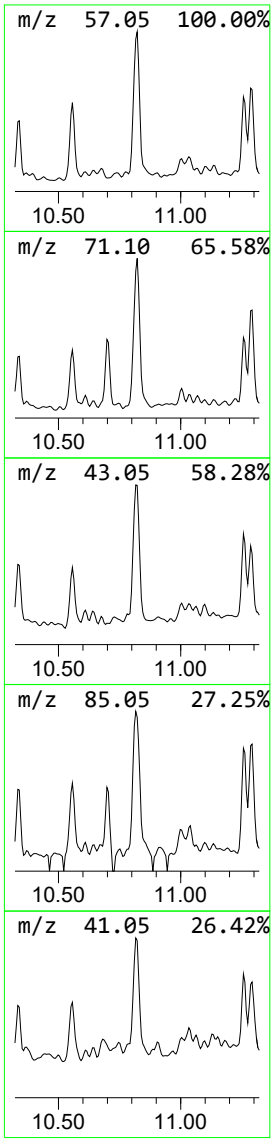
****

Peak Number 4 Tridecane, 5-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	2.09 ng	46113	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80
3	Tridecane	184	C13H28	000629-50-5	74
4	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	72
5	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	72





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Sample : Q2458-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-60

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

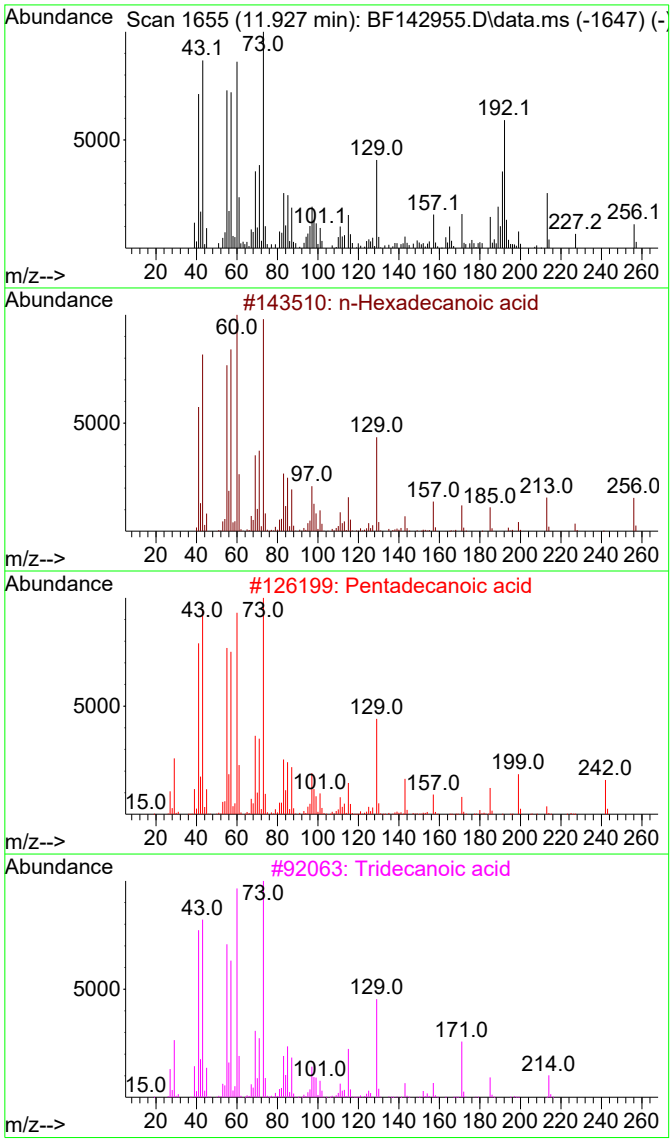
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

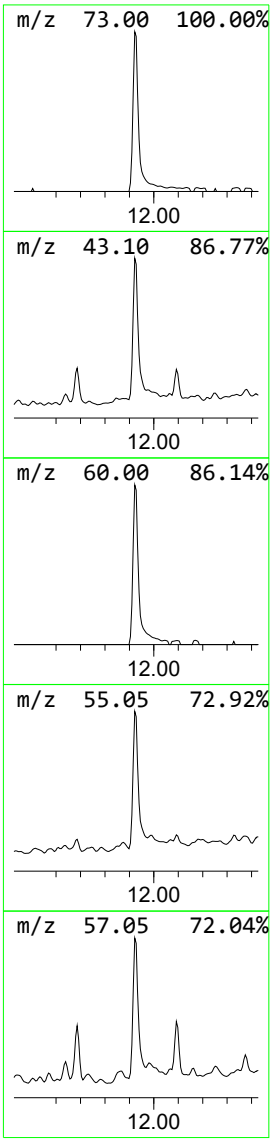
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	9.24 ng	204314	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	78
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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ClientSampleId :
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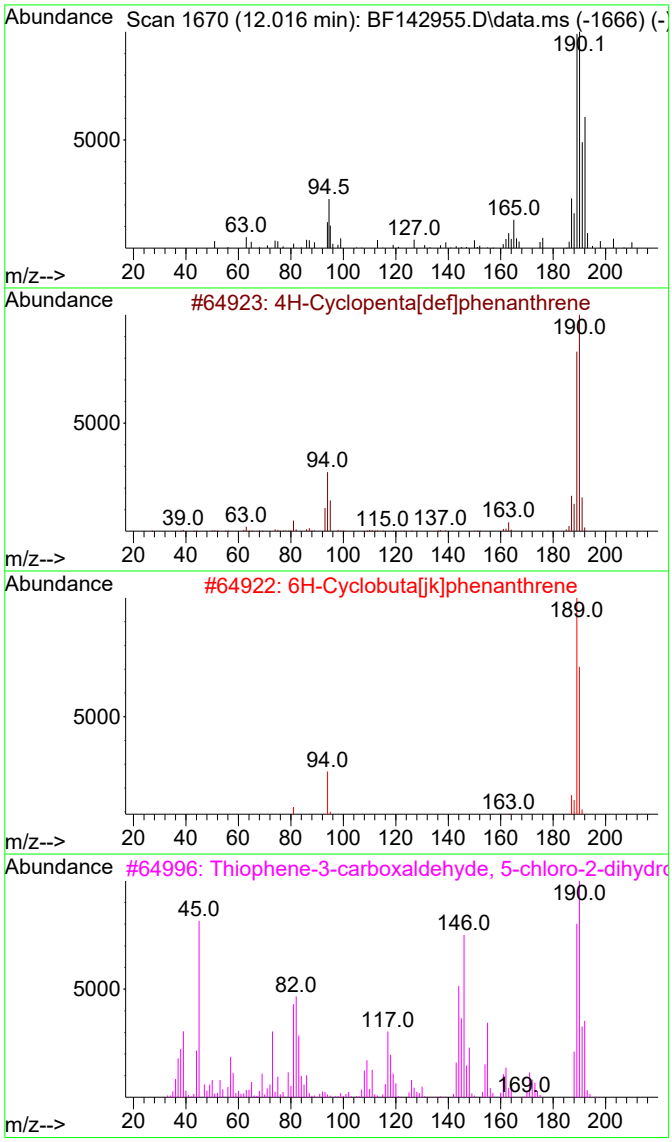
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

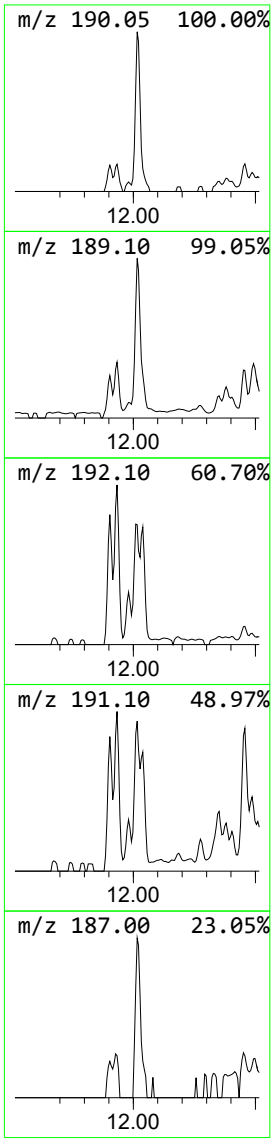
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	2.78 ng	61379	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	45
5	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070125\
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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
2-Pentanone, 4-...	5.075	5.8	ng	63672	1	6.875	220985	20.0
Biphenylene	9.775	2.1	ng	30643	3	9.910	289442	20.0
Benzophenone	10.622	5.4	ng	78555	3	9.910	289442	20.0
Tridecane, 5-pr...	10.822	2.1	ng	46113	4	11.404	442294	20.0
n-Hexadecanoic ...	11.928	9.2	ng	204314	4	11.404	442294	20.0
4H-Cyclopenta[d...	12.016	2.8	ng	61379	4	11.404	442294	20.0