LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142413.D
Acq On : 16 May 2025 01:27
Operator : RC/JU
Sample : Q1982-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

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-BF050525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	489	497	508	rBV	217149	337308	9.84%	1.185%
2	5.516	559	565	570	rBV	2131006	2829159	82.49%	9.940%
3	6.522	730	736	754	rVB	2123199	2928263	85.38%	10.288%
4	6.904	796	801	806	rVB	810517	1003875	29.27%	3.527%
5	7.463	885	896	901	rBV	1455304	1888266	55.06%	6.634%
6	7.710	935	938	944	rVB	42381	55940	1.63%	0.197%
7	8.186	1012	1019	1026	rBV	1013093	1336891	38.98%	4.697%
8	9.257	1196	1201	1206	rBV	2762873	3429600	100.00%	12.050%
9	9.339	1210	1215	1222	rBV2	36321	59580	1.74%	0.209%
10	9.592	1255	1258	1261	rVV	35088	49813	1.45%	0.175%
11	9.651	1265	1268	1275	rVV4	32266	57317	1.67%	0.201%
12	9.710	1275	1278	1288	rVB2	23566	50005	1.46%	0.176%
13	9.798	1289	1293	1298	rBV	52798	67267	1.96%	0.236%
14	9.863	1300	1304	1310	rVV2	24982	35176	1.03%	0.124%
15	9.939	1310	1317	1321	rVV	1039091	1340078	39.07%	4.708%
16	9.969	1321	1322	1330	rVB	92299	86340	2.52%	0.303%
17	10.139	1346	1351	1355	rVB	71098	91929	2.68%	0.323%
18	10.486	1405	1410	1416	rVB	131749	177207	5.17%	0.623%
19	10.651	1433	1438	1444	rVB2	186981	254464	7.42%	0.894%
20	10.727	1445	1451	1456	rBV	1295797	1735132	50.59%	6.096%
21	10.845	1466	1471	1478	rVB2	46698	81348	2.37%	0.286%
22	11.027	1498	1502	1505	rBV2	29156	43781	1.28%	0.154%
23	11.286	1541	1546	1548	rBV2	25546	40621	1.18%	0.143%
24	11.322	1548	1552	1558	rVB2	52893	77935	2.27%	0.274%
25	11.427	1564	1570	1578	rBV2	842363	1431907	41.75%	5.031%
26	11.498	1578	1582	1586	rVV	98314	120230	3.51%	0.422%
27	11.657	1605	1609	1615	rBV5	17945	38422	1.12%	0.135%
28	11.951	1651	1659	1664	rBV3	331395	574087	16.74%	2.017%
29	12.039	1670	1674	1682	rVB	152896	259914	7.58%	0.913%
30	12.222	1698	1705	1715	rVB3	45818	111961	3.26%	0.393%
31	12.474	1745	1748	1751	rBV	49181	62221	1.81%	0.219%
32	12.510	1751	1754	1760	rVB2	46318	69631	2.03%	0.245%
33	12.639	1771	1776	1780	rBV	557595	690432	20.13%	2.426%
34	12.680	1780	1783	1788	rVV5	25163	37803	1.10%	0.133%
35	12.733	1788	1792	1798	rVV2	58277	83422	2.43%	0.293%
36	12.869	1809	1815	1821	rVB	522887	755258	22.02%	2.654%

LSC Area Percent Report

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Acq On : 16 May 2025 01:27
Operator : RC/JU
Sample : Q1982-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

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-BF050525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.010	1834	1839	1846	rVB	2066979	2672418	77.92%	9.389%
38	13.086	1848	1852	1858	rVV3	55687	92186	2.69%	0.324%
39	13.192	1864	1870	1874	rVB	114783	186144	5.43%	0.654%
40	13.263	1879	1882	1885	rVV	90224	110461	3.22%	0.388%
41	13.298	1885	1888	1896	rVB2	77856	110278	3.22%	0.387%
42	13.392	1901	1904	1907	rBV	50997	56454	1.65%	0.198%
43	13.910	1988	1992	2002	rVB3	146426	264685	7.72%	0.930%
44	14.063	2013	2018	2030	rBV2	766593	1439227	41.96%	5.057%
45	15.121	2194	2198	2206	rVB	179501	387952	11.31%	1.363%
46	15.492	2258	2261	2267	rVB	124499	163263	4.76%	0.574%
47	15.557	2268	2272	2284	rVB	367774	686458	20.02%	2.412%

Sum of corrected areas: 28462109

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Instrument :
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ClientSampleId :
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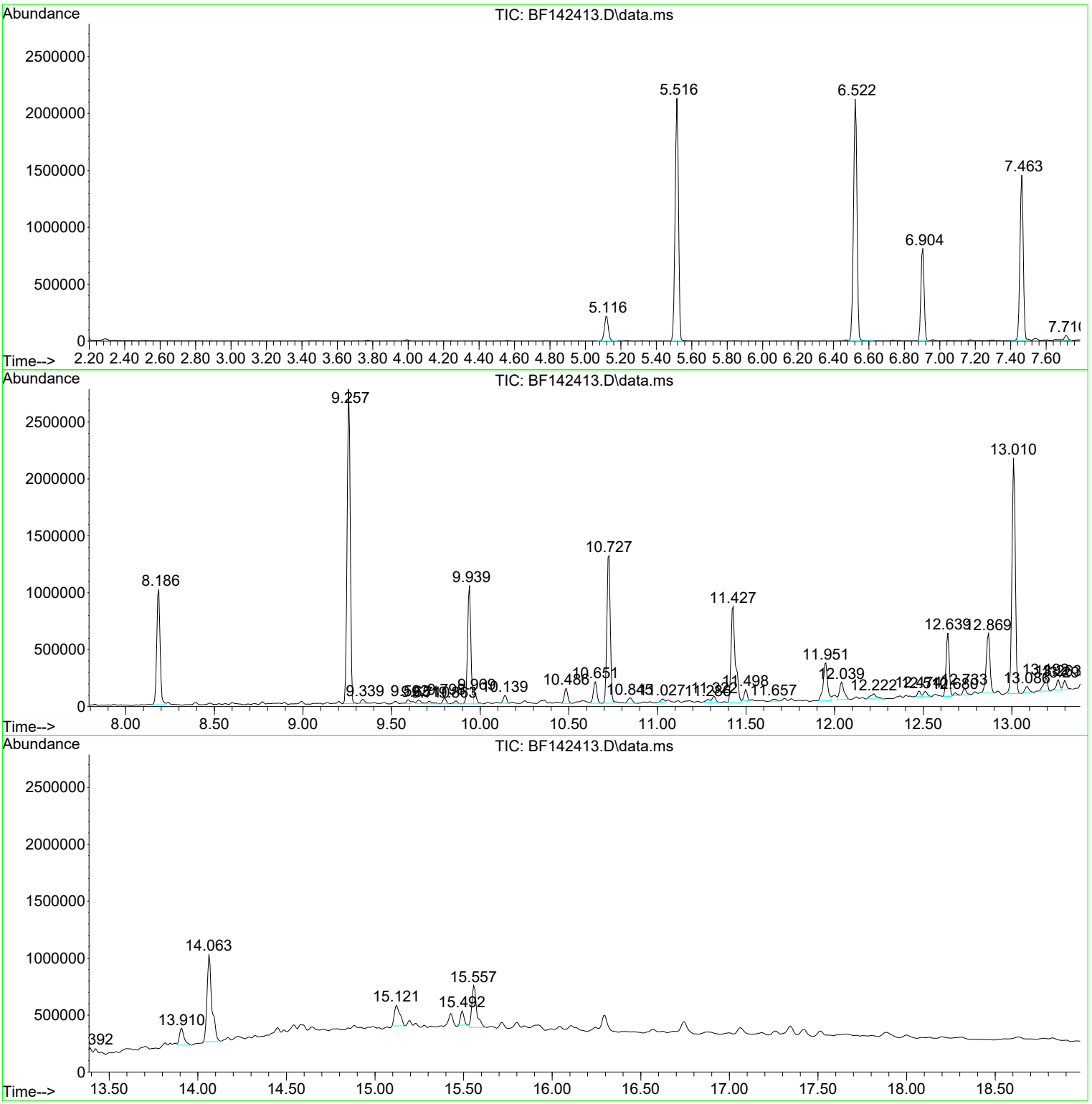
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142413.D
Acq On : 16 May 2025 01:27
Operator : RC/JU
Sample : Q1982-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

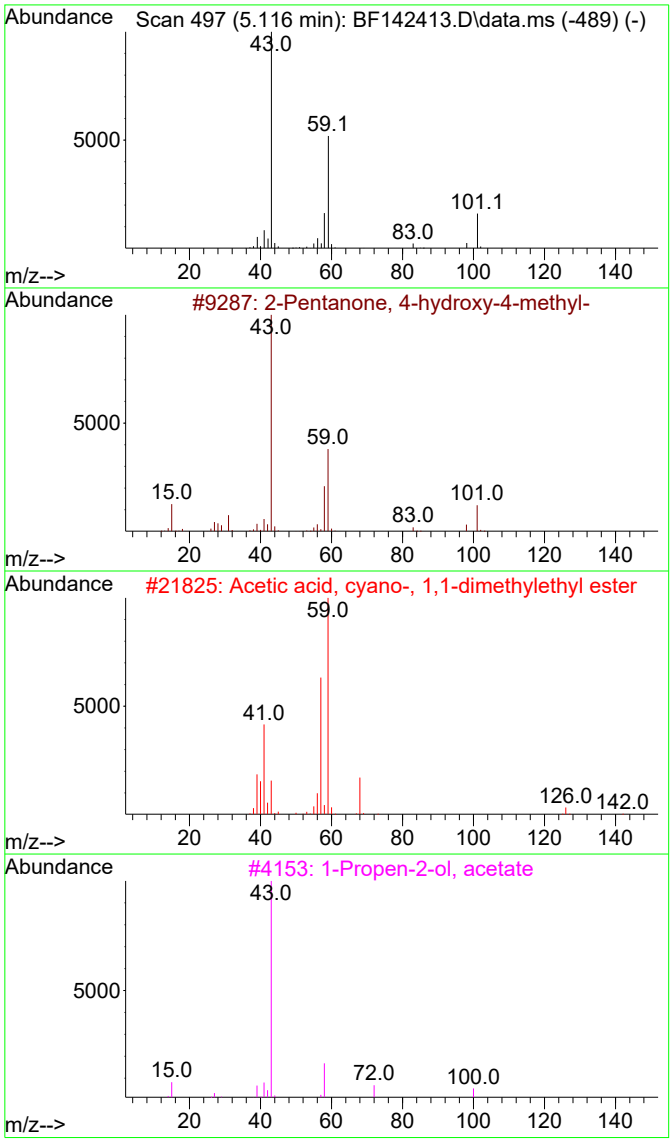
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

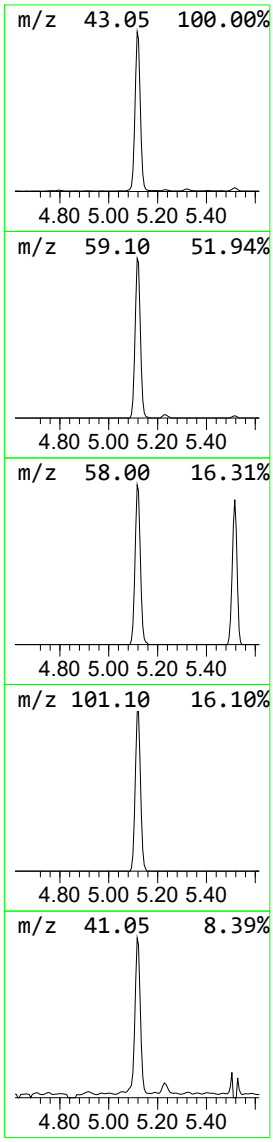
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	6.72 ng	337308	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142413.D
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

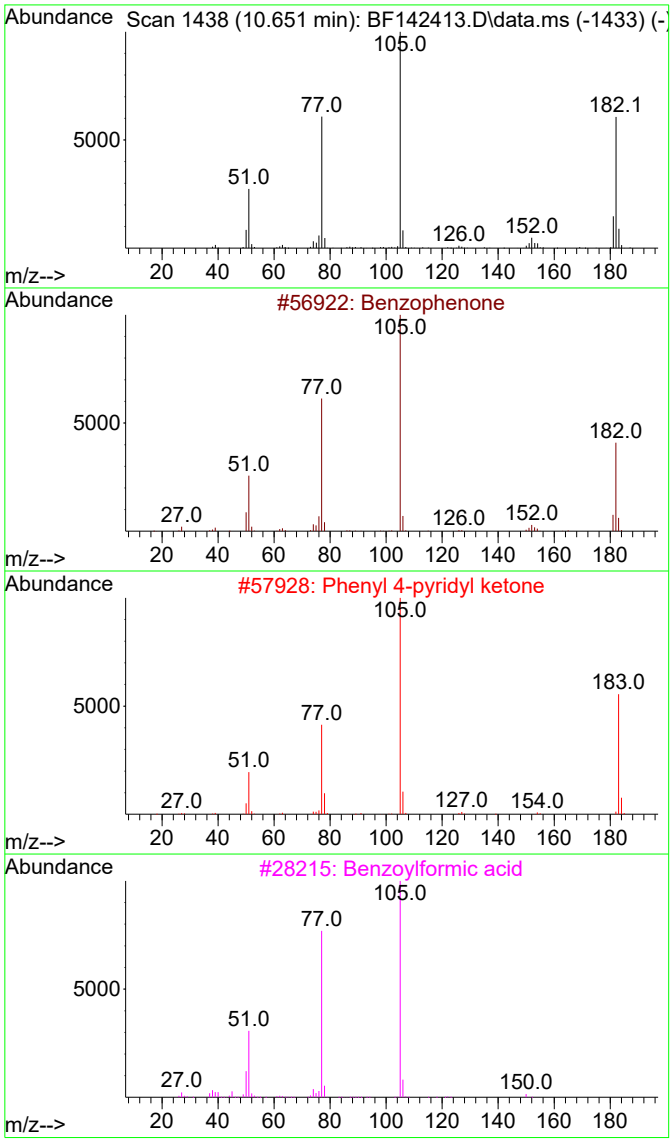
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

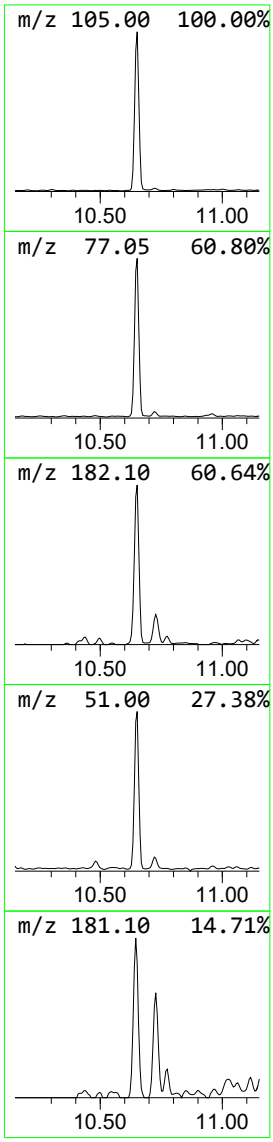
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	3.80 ng	254464	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
3	Benzoylformic acid	150	C8H6O3	000611-73-4	49
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142413.D
Acq On : 16 May 2025 01:27
Operator : RC/JU
Sample : Q1982-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

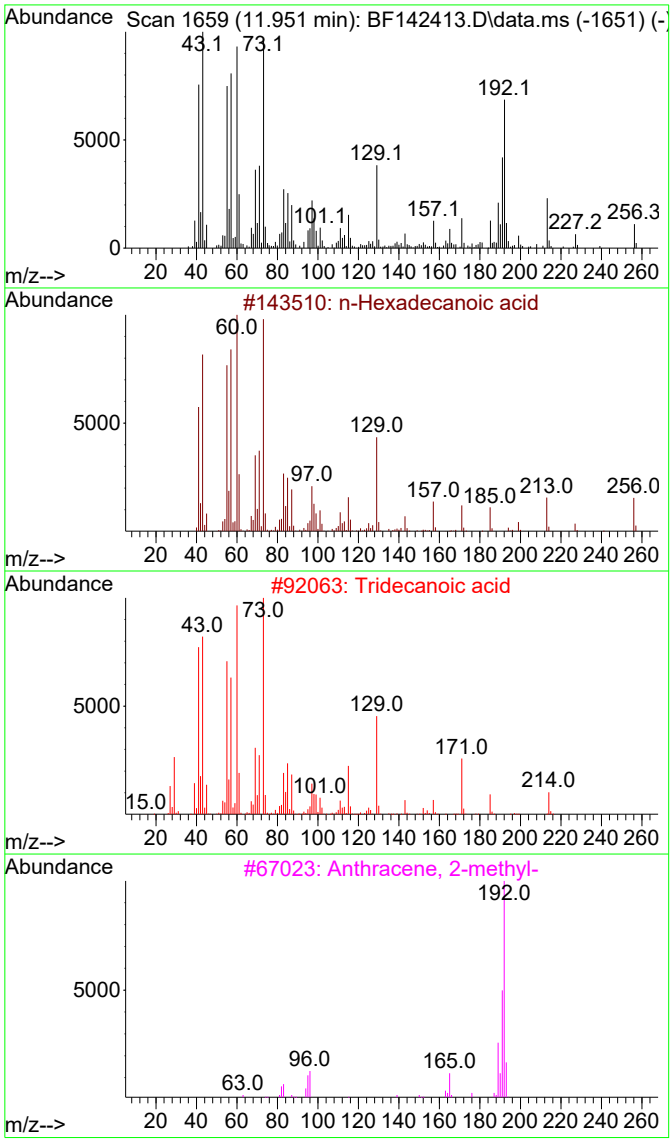
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

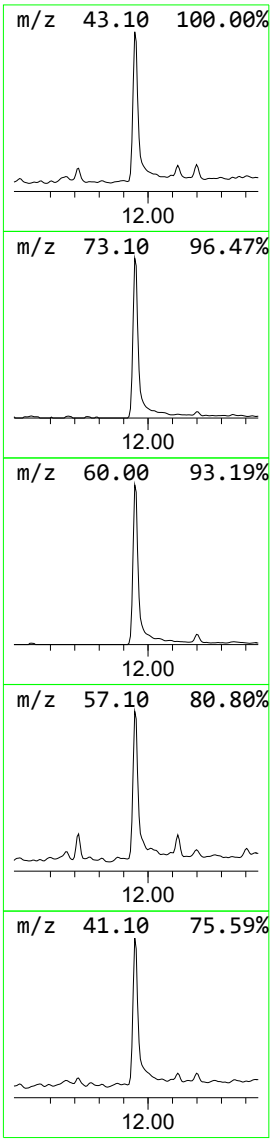
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	8.02 ng	574087	Phenanthrene-d10	11.427

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	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142413.D
Acq On : 16 May 2025 01:27
Operator : RC/JU
Sample : Q1982-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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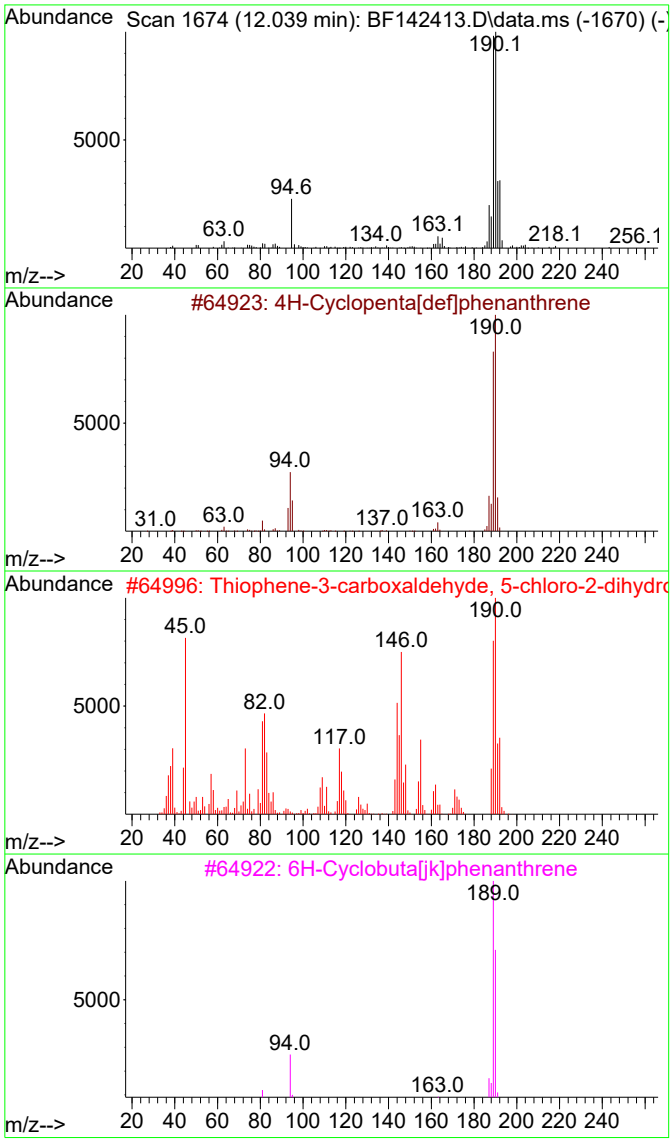
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

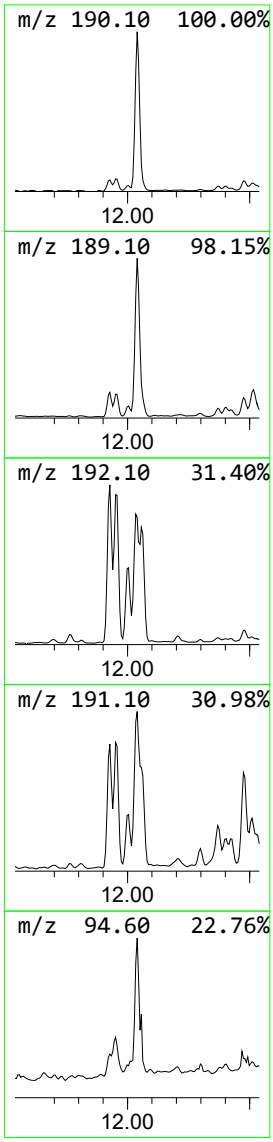
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	3.63 ng	259914	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142413.D
Acq On : 16 May 2025 01:27
Operator : RC/JU
Sample : Q1982-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

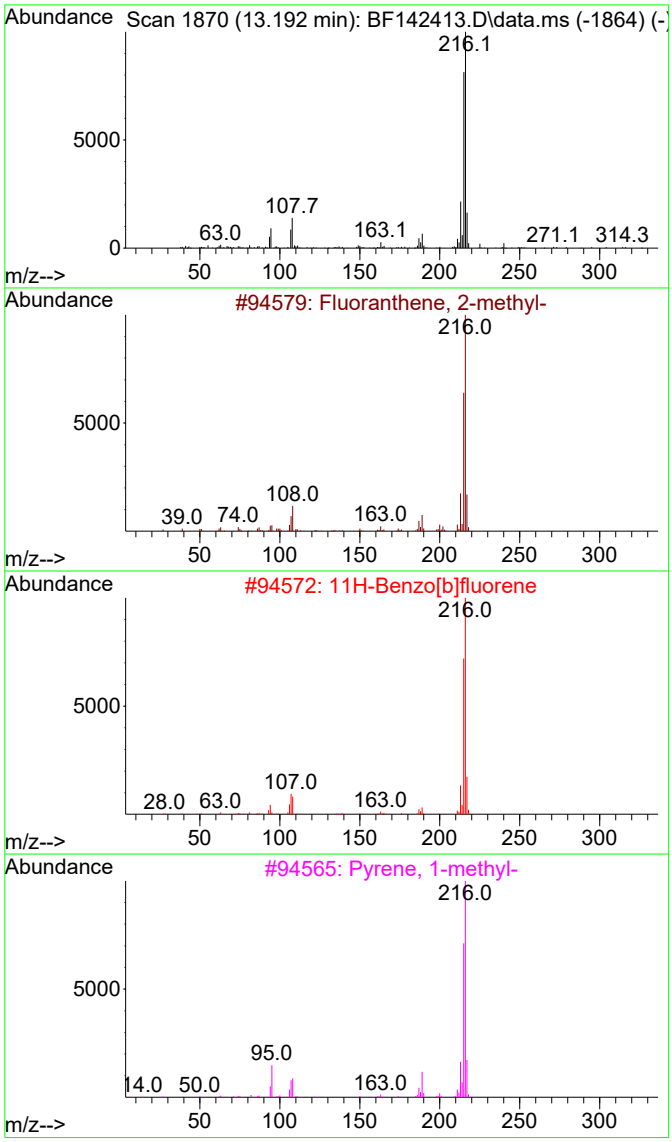
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

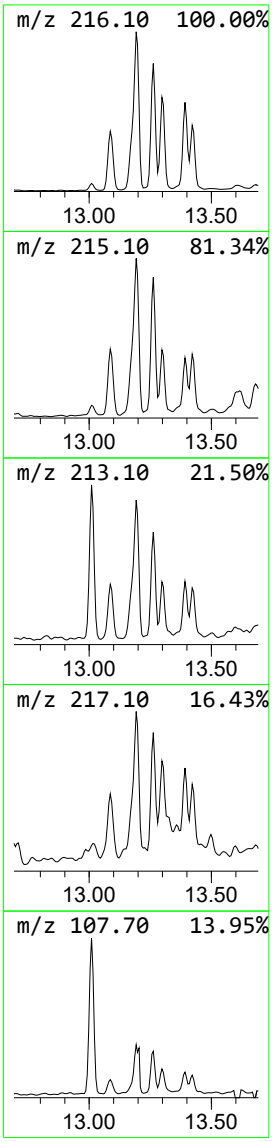
****

Peak Number 5 Fluoranthene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	2.59 ng	186144	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	96
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





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BNA_F
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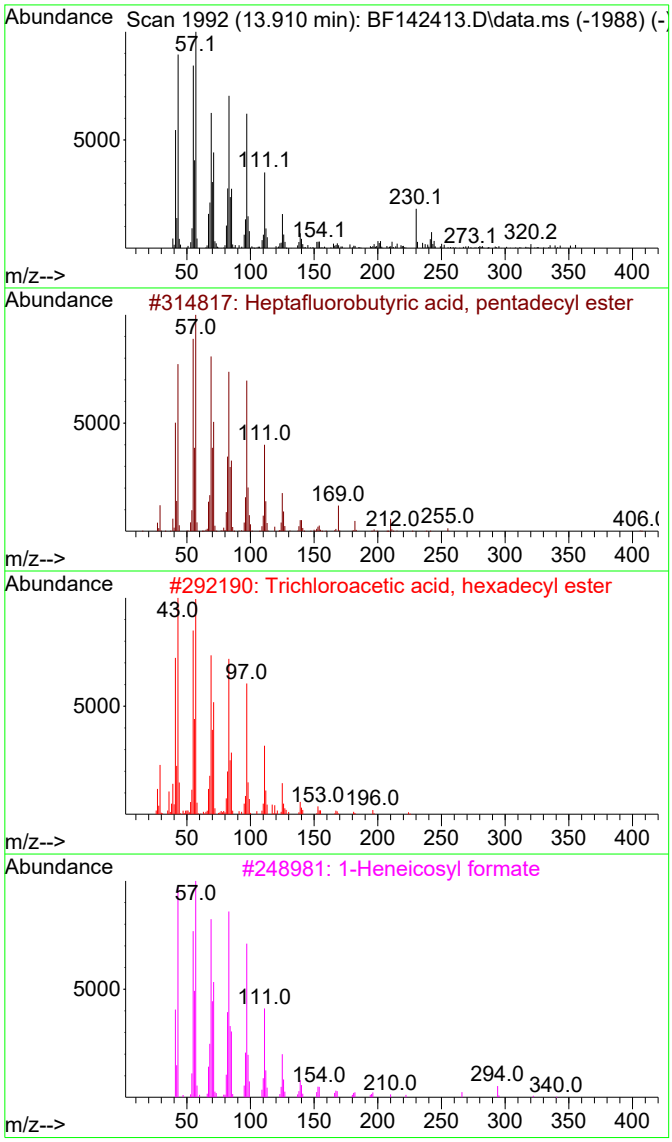
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

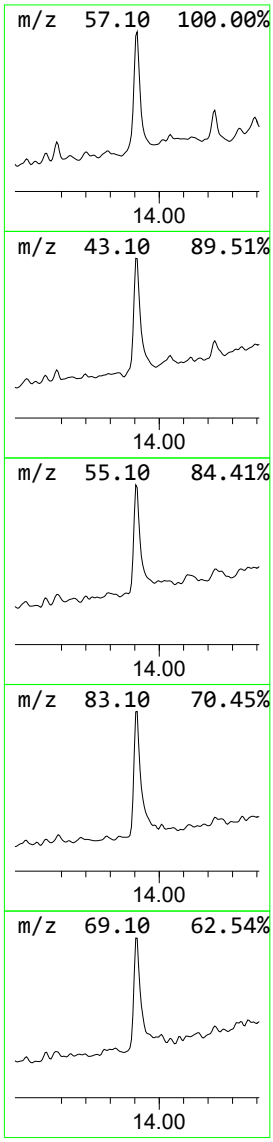
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.68 ng	264685	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142413.D
Acq On : 16 May 2025 01:27
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Sample : Q1982-04
Misc :
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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
2-Pentanone, 4-...	5.116	6.7	ng	337308	1	6.904	1003880	20.0
Benzophenone	10.651	3.8	ng	254464	3	9.939	1340080	20.0
n-Hexadecanoic ...	11.951	8.0	ng	574087	4	11.427	1431910	20.0
4H-Cyclopenta[d...	12.039	3.6	ng	259914	4	11.427	1431910	20.0
Fluoranthene, 2...	13.192	2.6	ng	186144	5	14.068	1439230	20.0
Heptafluorobuty...	13.910	3.7	ng	264685	5	14.068	1439230	20.0