LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112923\
Data File : BF136291.D
Acq On : 29 Nov 2023 19:15
Operator : CG\JU
Sample : 05503-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136291.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	497	502	508	rVB	36472	44232	2.11%	0.216%
2	5.440	565	570	573	rBV	2324407	2030582	96.70%	9.901%
3	6.087	677	680	684	rVB	68758	59893	2.85%	0.292%
4	6.434	734	739	742	rBV	2149493	1974327	94.02%	9.627%
5	6.634	770	773	785	rBV	46086	59979	2.86%	0.292%
6	6.804	798	802	805	rBV	871092	662675	31.56%	3.231%
7	6.916	818	821	824	rVB	42744	33870	1.61%	0.165%
8	7.363	892	897	900	rBV	1455190	1261123	60.05%	6.149%
9	8.081	1015	1019	1022	rBV	1093637	873887	41.61%	4.261%
10	9.157	1198	1202	1205	rBV	2782653	2099966	100.00%	10.239%
11	9.280	1218	1223	1237	rVB	1415944	1394865	66.42%	6.801%
12	9.810	1310	1313	1315	rBV	67778	70132	3.34%	0.342%
13	9.839	1315	1318	1321	rVB	978561	879595	41.89%	4.289%
14	10.627	1448	1452	1455	rBV	1243271	1036626	49.36%	5.054%
15	10.816	1479	1484	1496	rVB2	22514	54047	2.57%	0.264%
16	10.922	1496	1502	1507	rBV	30681	46099	2.20%	0.225%
17	10.980	1507	1512	1517	rBV3	21363	37171	1.77%	0.181%
18	11.327	1567	1571	1573	rBV	885199	704399	33.54%	3.435%
19	11.351	1573	1575	1578	rVV	217781	164786	7.85%	0.803%
20	11.404	1580	1584	1587	rVB	33592	35091	1.67%	0.171%
21	11.492	1596	1599	1604	rVB	29419	37150	1.77%	0.181%
22	11.863	1659	1662	1667	rBV2	221627	218562	10.41%	1.066%
23	11.939	1672	1675	1678	rBV2	39150	42614	2.03%	0.208%
24	12.151	1709	1711	1715	rVB2	31660	29878	1.42%	0.146%
25	12.439	1758	1760	1763	rVB	64713	51816	2.47%	0.253%
26	12.468	1763	1765	1769	rVB3	27338	28213	1.34%	0.138%
27	12.545	1772	1778	1781	rBV	382467	331276	15.78%	1.615%
28	12.586	1781	1785	1788	rBV	85277	74606	3.55%	0.364%
29	12.657	1792	1797	1802	rBV3	40933	57246	2.73%	0.279%
30	12.774	1809	1817	1820	rBV	357753	358025	17.05%	1.746%
31	12.827	1824	1826	1830	rVB5	28501	28510	1.36%	0.139%
32	12.921	1839	1842	1846	rBV	1769993	1533045	73.00%	7.475%
33	12.992	1850	1854	1858	rBV3	34516	46943	2.24%	0.229%
34	13.080	1866	1869	1870	rBV3	30736	27646	1.32%	0.135%
35	13.104	1871	1873	1876	rVB2	40505	38651	1.84%	0.188%
36	13.168	1880	1884	1887	rBV2	39405	45200	2.15%	0.220%

LSC Area Percent Report

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Sample : 05503-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

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-BF112723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.210	1887	1891	1894	rBV2	47403	53356	2.54%	0.260%
38	13.304	1903	1907	1910	rBV	27679	29460	1.40%	0.144%
39	13.510	1935	1942	1945	rBV4	43768	51672	2.46%	0.252%
40	13.615	1957	1960	1964	rVB	33000	38239	1.82%	0.186%
41	13.698	1971	1974	1976	rBV	113553	98750	4.70%	0.481%
42	13.721	1976	1978	1982	rVB2	35995	39942	1.90%	0.195%
43	13.757	1982	1984	1986	rBV	36601	28648	1.36%	0.140%
44	13.780	1986	1988	1992	rVB3	42141	48761	2.32%	0.238%
45	13.821	1992	1995	2000	rBV4	50206	82916	3.95%	0.404%
46	13.857	2000	2001	2013	rVB4	48900	101404	4.83%	0.494%
47	13.980	2017	2022	2025	rBV2	774870	835662	39.79%	4.075%
48	14.004	2025	2026	2029	rVB	168003	95203	4.53%	0.464%
49	14.080	2035	2039	2042	rVB3	28177	35220	1.68%	0.172%
50	14.162	2050	2053	2056	rVB3	43965	42998	2.05%	0.210%
51	14.368	2085	2088	2092	rVB	39682	35470	1.69%	0.173%
52	14.404	2092	2094	2097	rBV3	31889	31407	1.50%	0.153%
53	14.468	2101	2105	2107	rBV2	54586	58490	2.79%	0.285%
54	14.568	2120	2122	2128	rVB5	41034	61496	2.93%	0.300%
55	14.627	2128	2132	2136	rBV	445817	423511	20.17%	2.065%
56	14.674	2137	2140	2143	rVV5	25112	31373	1.49%	0.153%
57	14.762	2152	2155	2156	rBV3	26314	29816	1.42%	0.145%
58	14.780	2156	2158	2162	rVB2	48939	48779	2.32%	0.238%
59	14.857	2167	2171	2177	rVB3	125268	144700	6.89%	0.706%
60	15.027	2195	2200	2203	rBV	200721	306556	14.60%	1.495%
61	15.133	2211	2218	2222	rVB3	86754	124598	5.93%	0.608%
62	15.333	2248	2252	2257	rVB	114577	141685	6.75%	0.691%
63	15.398	2259	2263	2269	rVB	101483	127655	6.08%	0.622%
64	15.462	2269	2274	2278	rBV	474599	582178	27.72%	2.839%
65	15.980	2356	2362	2368	rBV2	49428	89796	4.28%	0.438%
66	16.509	2448	2452	2457	rVB5	22968	37418	1.78%	0.182%
67	16.951	2522	2527	2536	rVB2	39406	92003	4.38%	0.449%
68	17.139	2555	2559	2564	rVB6	20866	34461	1.64%	0.168%
69	17.409	2601	2605	2611	rVB	26439	52725	2.51%	0.257%

Sum of corrected areas: 20509074

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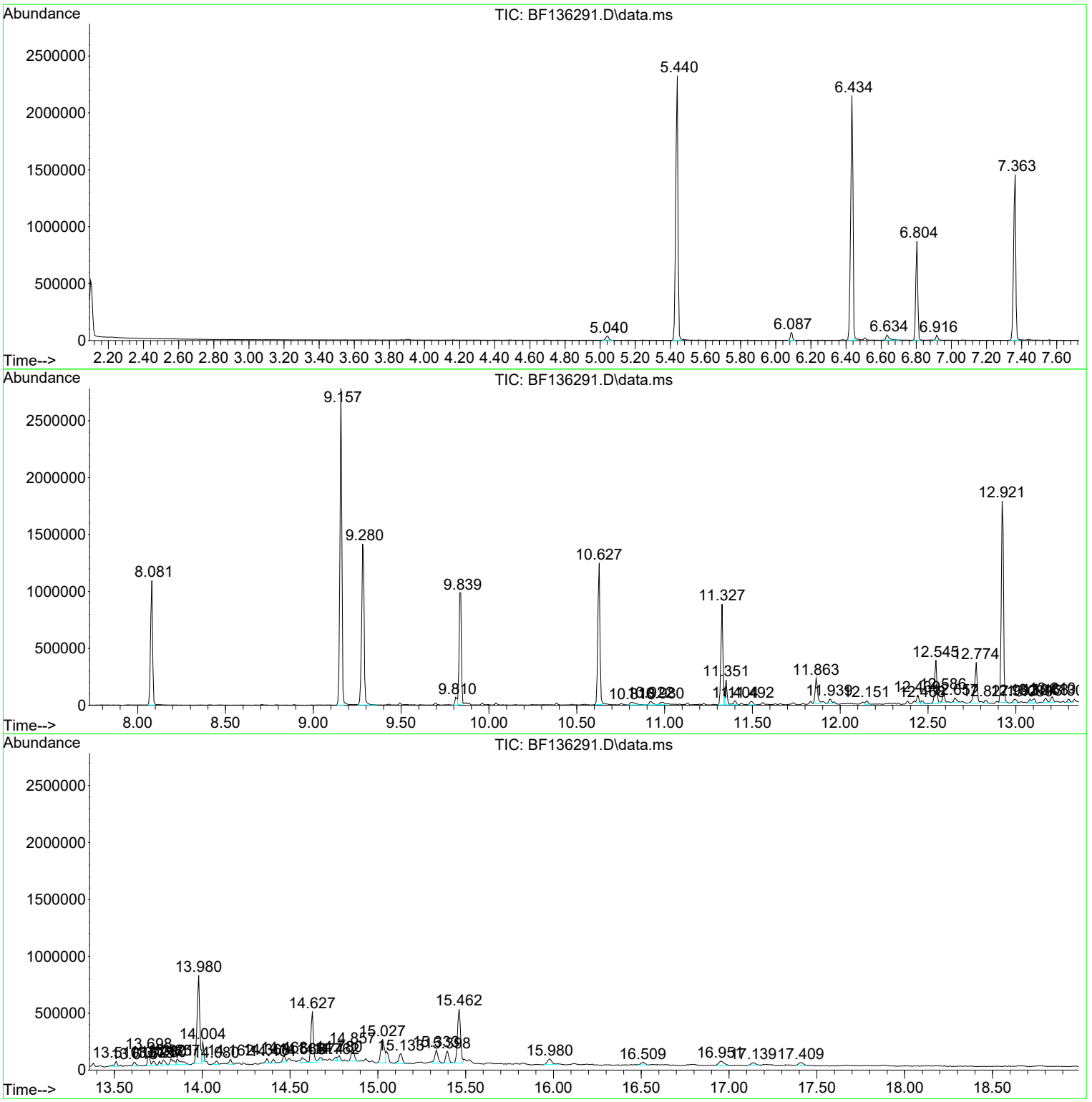
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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\BF112923\
Data File : BF136291.D
Acq On : 29 Nov 2023 19:15
Operator : CG\JU
Sample : 05503-04
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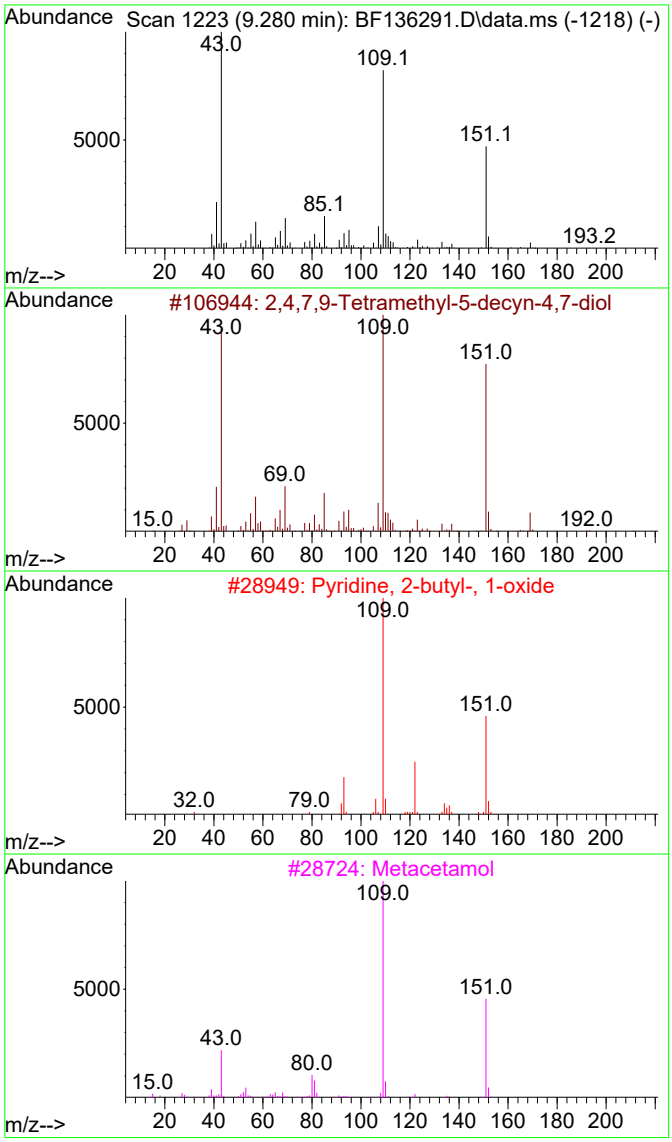
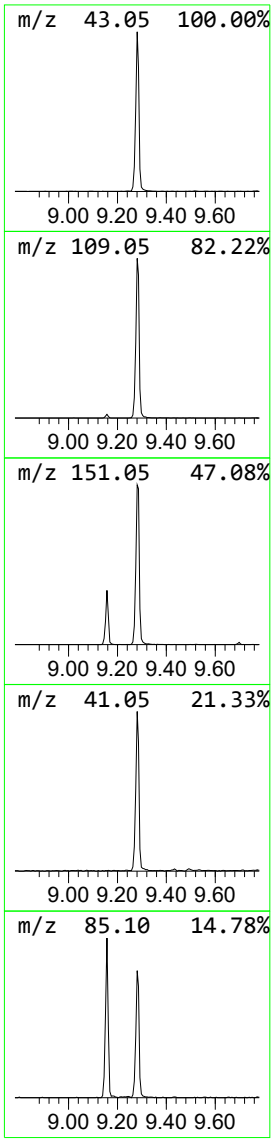
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.280	31.72 ng	1394870	Acenaphthene-d10	9.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	Metacetamol	151	C8H9NO2	000621-42-1	59
4	Acetaminophen	151	C8H9NO2	000103-90-2	59
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	45





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Data File : BF136291.D
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Operator : CG\JU
Sample : 05503-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

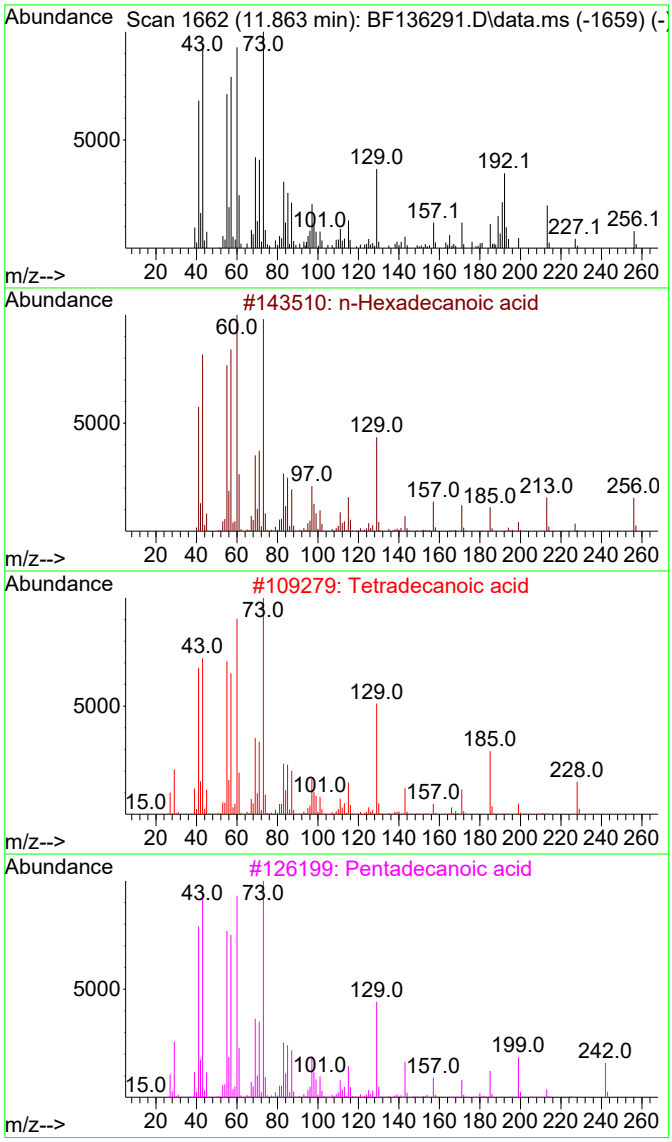
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

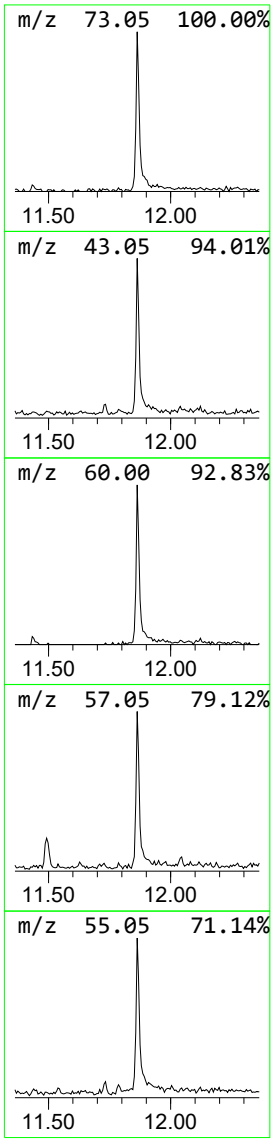
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	6.21 ng	218562	Phenanthrene-d10	11.327

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	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Sample : 05503-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

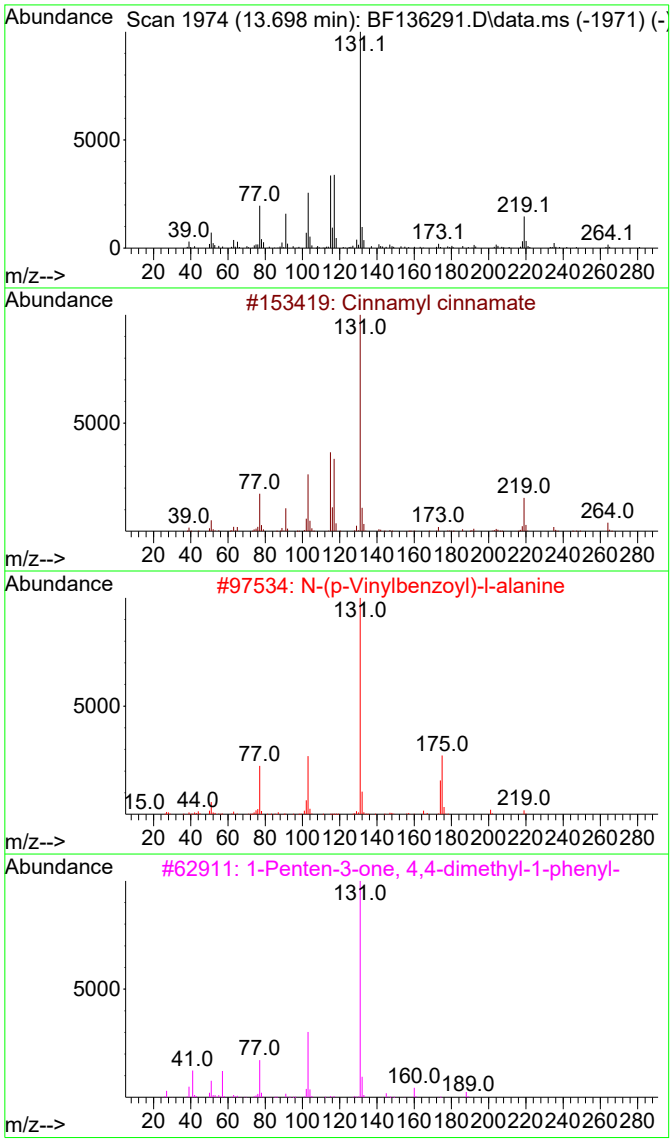
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

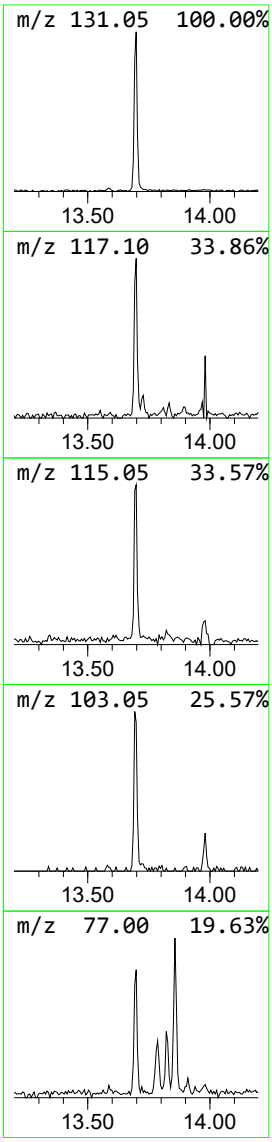
****

Peak Number 3 Cinnamyl cinnamate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.698	2.36 ng	98750	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	50
3	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	50
4	1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	50
5	Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112923\
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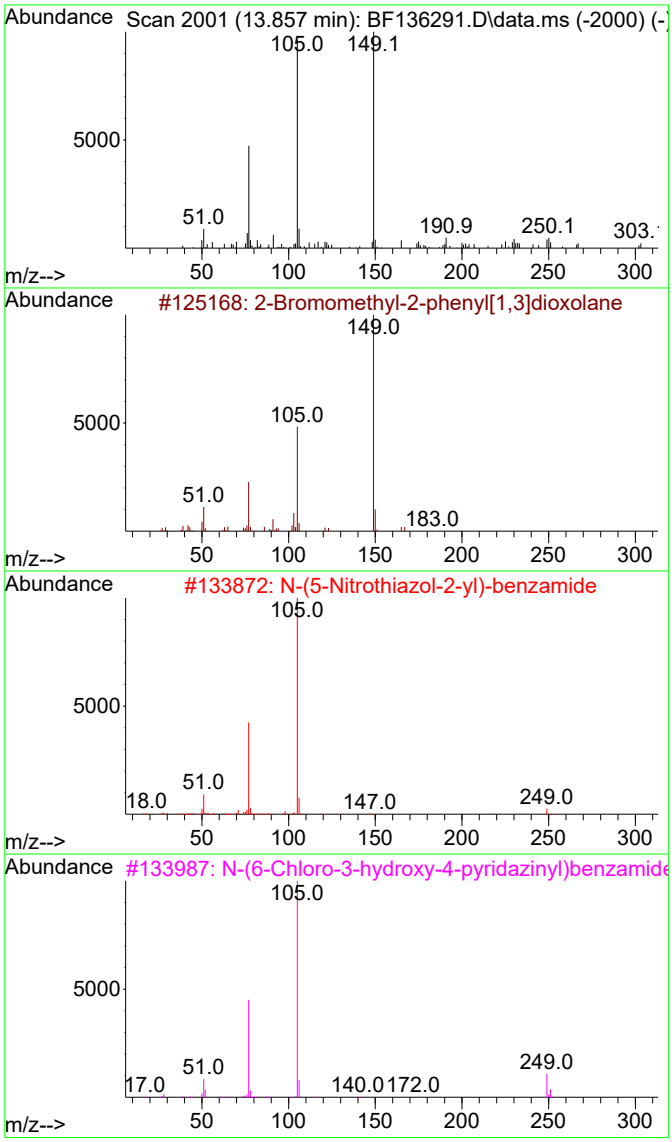
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

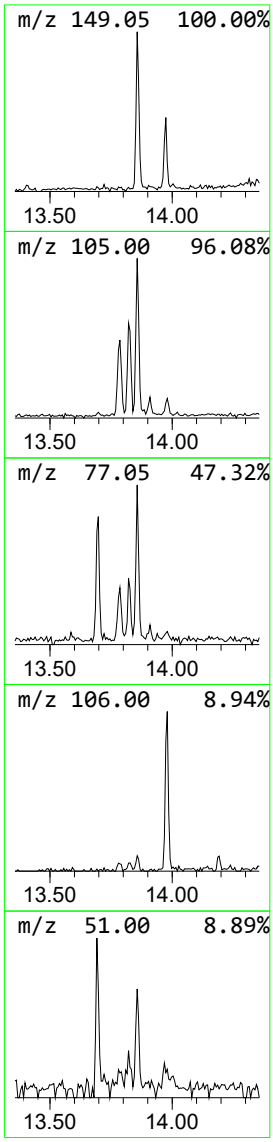
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Bromomethyl-2-phenyl[1,3]... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.43 ng	101404	Chrysene-d12	13.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromomethyl-2-phenyl[1,3]dioxo...	242	C10H11BrO2	003418-21-1	50
2	N-(5-Nitrothiazol-2-yl)-benzamide	249	C10H7N3O3S	064398-84-1	30
3	N-(6-Chloro-3-hydroxy-4-pyridazi...	249	C11H8ClN3O2	117892-39-4	27
4	Benzamide, N-(5-acetyl-1,2,3-tri...	230	C11H10N4O2	129959-33-7	27
5	N-(5-Pyrimidinyl)benzamide, Ac d...	241	C13H11N3O2	1000504-27-8	25





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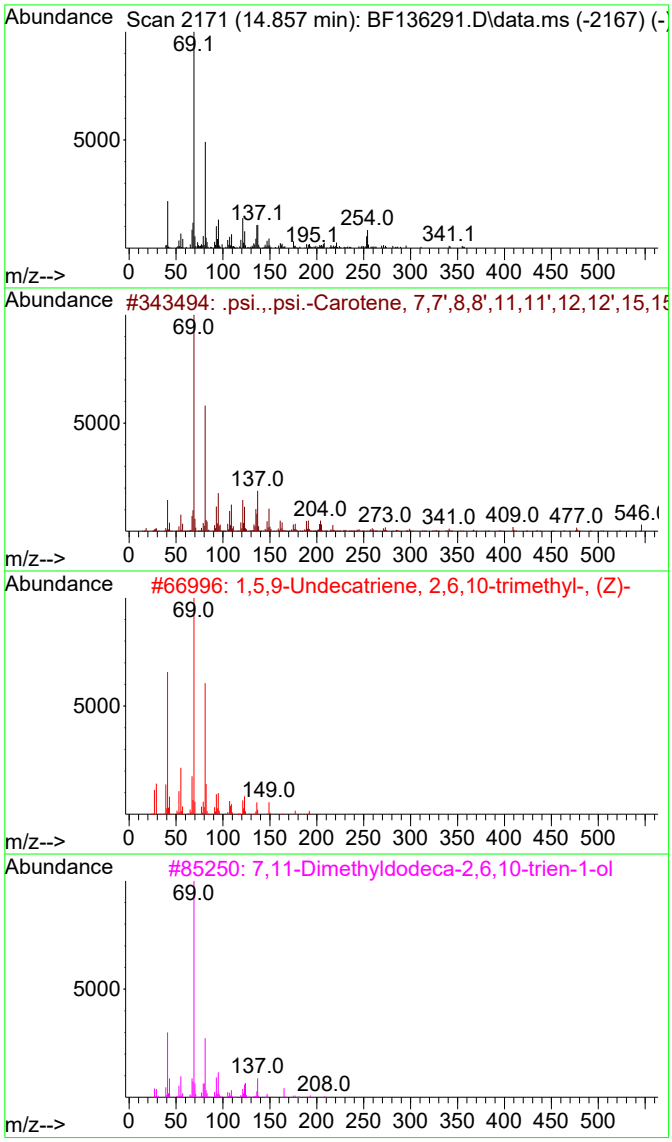
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

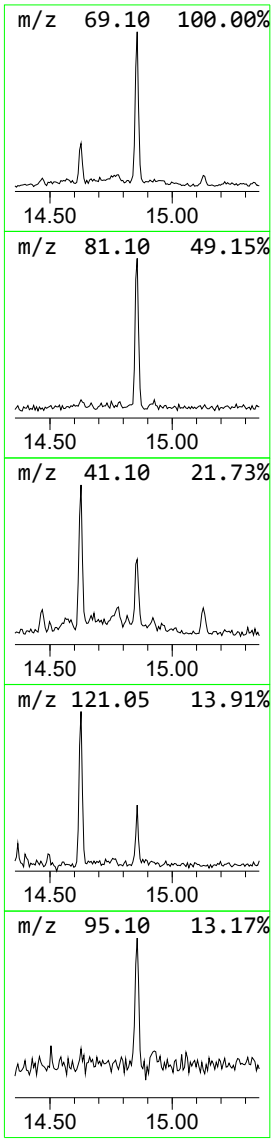
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 .psi.,.psi.-Carotene, 7,7',... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	4.97 ng	144700	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	Supraene	410	C30H50	007683-64-9	64
5	(Z)-all-trans-3,7,11-Trimethyl-2...	235	C15H25NO	123257-83-0	58





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

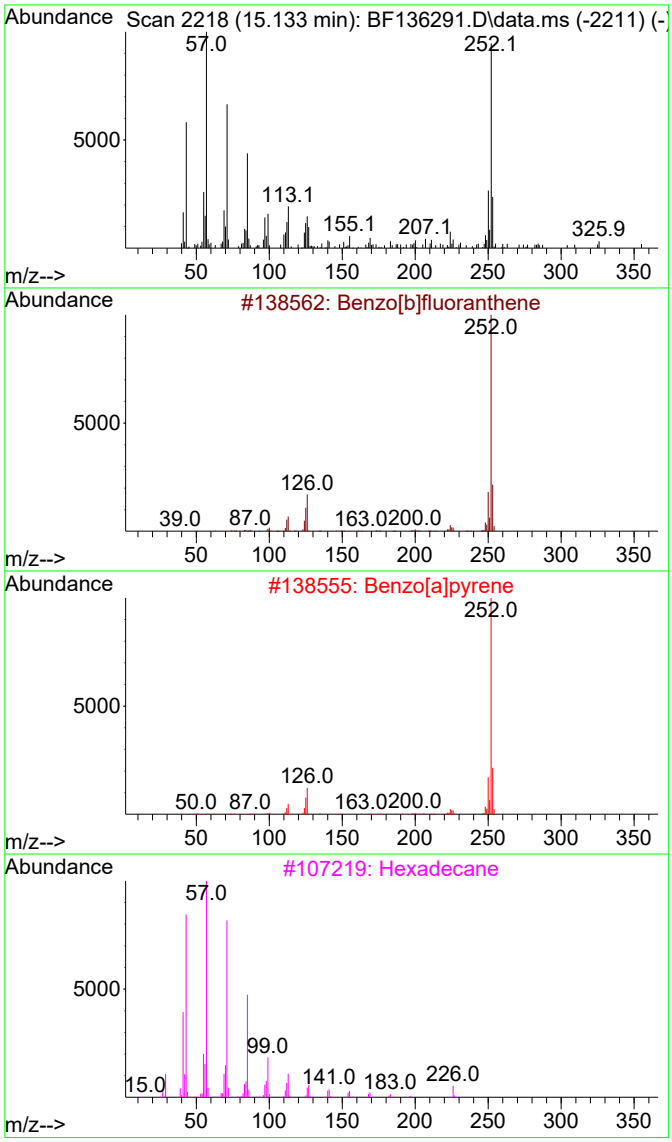
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

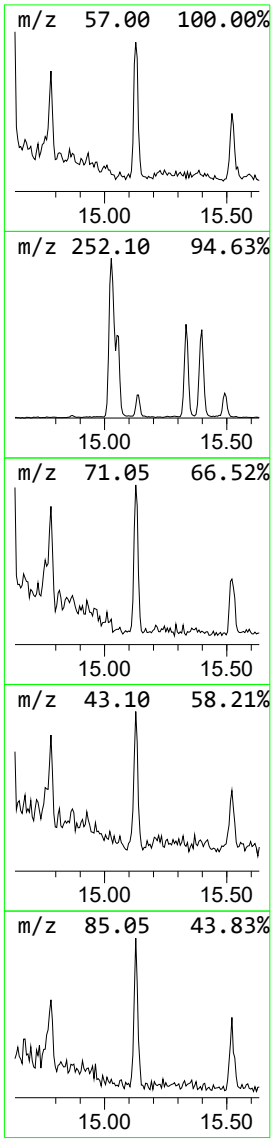
****

Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	4.28 ng	124598	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	78
2	Benzo[a]pyrene	252	C20H12	000050-32-8	76
3	Hexadecane	226	C16H34	000544-76-3	74
4	Benzo[e]pyrene	252	C20H12	000192-97-2	60
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112923\
Data File : BF136291.D
Acq On : 29 Nov 2023 19:15
Operator : CG\JU
Sample : 05503-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

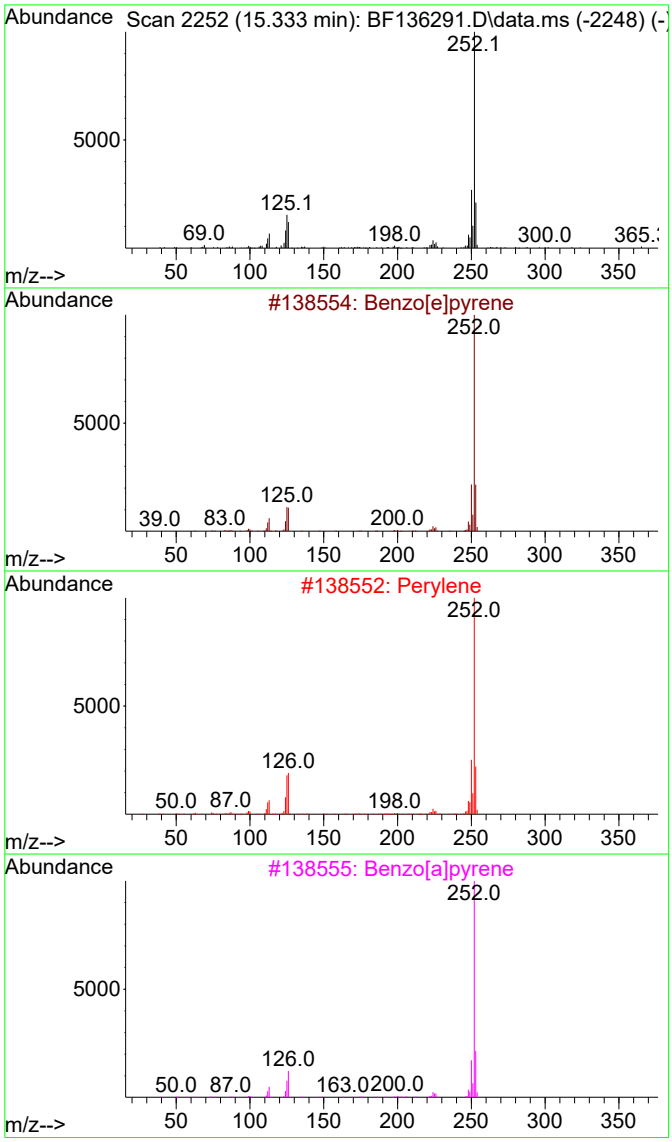
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

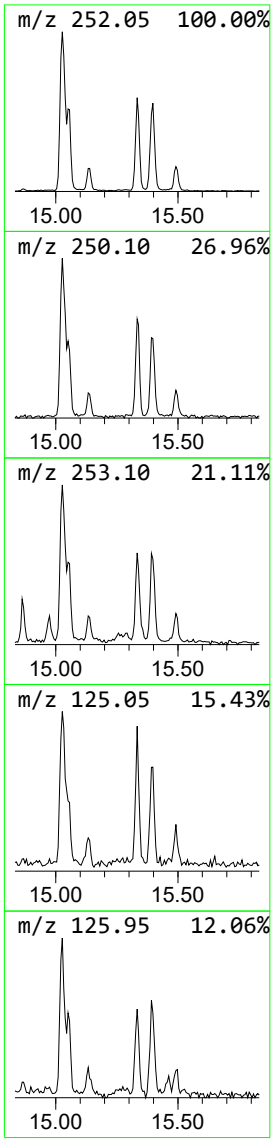
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	4.87 ng	141685	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Perylene	252	C20H12	000198-55-0	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112923\
Data File : BF136291.D
Acq On : 29 Nov 2023 19:15
Operator : CG\JU
Sample : 05503-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

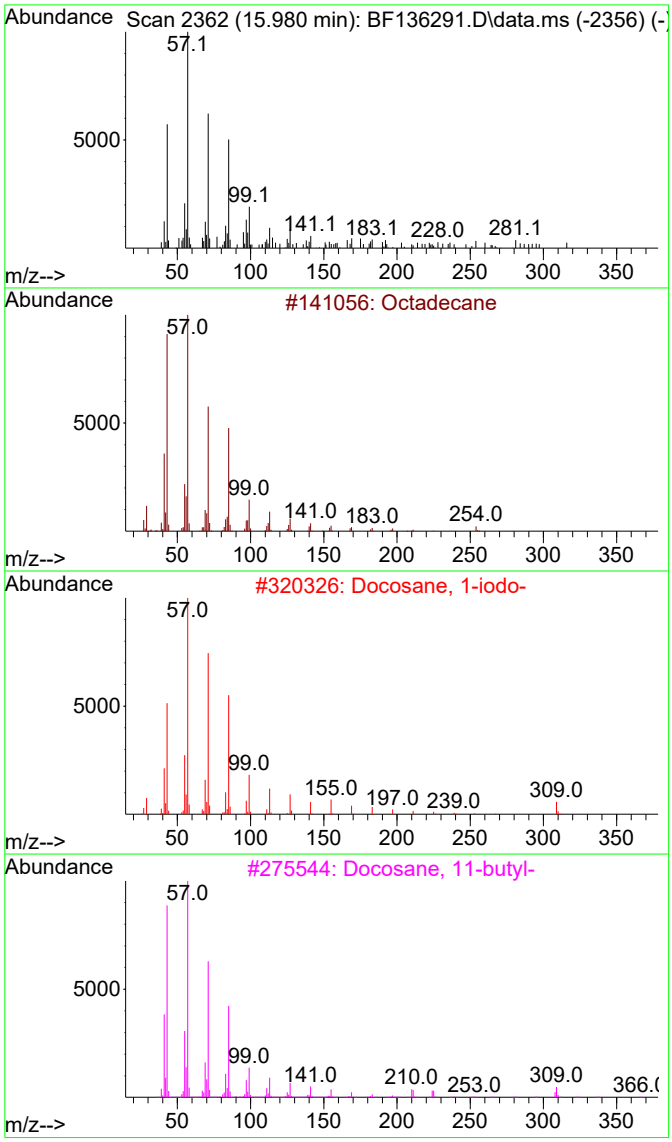
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

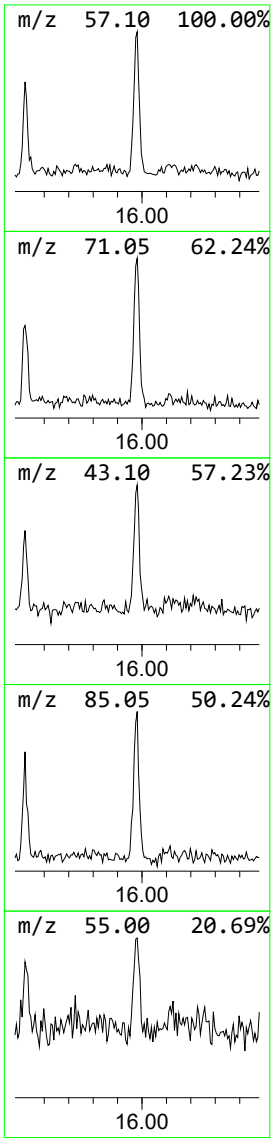
****

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	3.08 ng	89796	Perylene-d12	15.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
4	4-Methylheneicosane	310	C22H46	025117-29-7	86
5	Triacontane	422	C30H62	000638-68-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112923\
Data File : BF136291.D
Acq On : 29 Nov 2023 19:15
Operator : CG\JU
Sample : 05503-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112723.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
2,4,7,9-Tetrame...	9.280	31.7	ng	1394870	3	9.839	879595	20.0
n-Hexadecanoic ...	11.863	6.2	ng	218562	4	11.327	704399	20.0
Cinnamyl cinnamate	13.698	2.4	ng	98750	5	13.980	835662	20.0
2-Bromomethyl-2...	13.857	2.4	ng	101404	5	13.980	835662	20.0
.psi.,.psi.-Car...	14.857	5.0	ng	144700	6	15.462	582178	20.0
Hexadecane	15.133	4.3	ng	124598	6	15.462	582178	20.0
Benzo[e]pyrene	15.333	4.9	ng	141685	6	15.462	582178	20.0
Octadecane	15.980	3.1	ng	89796	6	15.462	582178	20.0